Trying 3106016892...Open

j

Welcome to STN International! Enter x:x LOGINID:ssspta1611hxl PASSWORD: TERMINAL (ENTER 1, 2, 3, OR ?):2

Species to EP 0786386.

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* * * * * * * * *
                     Welcome to STN International
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 IMSworld Pharmaceutical Company Directory name change
NEWS
      2 Sep 17
                 to PHARMASEARCH
                 Korean abstracts now included in Derwent World Patents
      3 Oct 09
NEWS
                 Index
NEWS 4 Oct 09 Number of Derwent World Patents Index updates increased
NEWS 5 Oct 15 Calculated properties now in the REGISTRY/ZREGISTRY File
NEWS 6 Oct 22 Over 1 million reactions added to CASREACT
NEWS 7
         Oct 22 DGENE GETSIM has been improved
NEWS 8 Oct 29 AAASD no longer available
NEWS 9
         Nov 19 New Search Capabilities USPATFULL and USPAT2
NEWS 10
         Nov 19
                 TOXCENTER(SM) - new toxicology file now available on STN
NEWS 11
         Nov 29 COPPERLIT now available on STN
NEWS 12
         Nov 29 DWPI revisions to NTIS and US Provisional Numbers
                 Files VETU and VETB to have open access
NEWS 13
         Nov 30
NEWS 14
         Dec 10 WPINDEX/WPIDS/WPIX New and Revised Manual Codes for 2002
NEWS 15
         Dec 10 DGENE BLAST Homology Search
NEWS 16 Dec 17 WELDASEARCH now available on STN
NEWS 17
         Dec 17 STANDARDS now available on STN
NEWS 18 Dec 17 New fields for DPCI
NEWS 19 Dec 19 CAS Roles modified
NEWS 20 Dec 19 1907-1946 data and page images added to CA and CAplus
NEWS 21
         Jan 25
                 BLAST(R) searching in REGISTRY available in STN on the Web
NEWS 22
                 Searching with the P indicator for Preparations
         Jan 25
NEWS 23
         Jan 29
                 FSTA has been reloaded and moves to weekly updates
NEWS 24
                 DKILIT now produced by FIZ Karlsruhe and has a new update
         Feb 01
                 frequency
              February 1 CURRENT WINDOWS VERSION IS V6.0d,
NEWS EXPRESS
              CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
              AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS INTER
              General Internet Information
NEWS LOGIN
              Welcome Banner and News Items
NEWS PHONE
              Direct Dial and Telecommunication Network Access to STN
NEWS WWW
              CAS World Wide Web Site (general information)
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FILE 'HOME' ENTERED AT 10:53:33 ON 07 FEB 2002

=> fil caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.15 0.15

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 10:54:12 ON 07 FEB 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 7 Feb 2002 VOL 136 ISS 6 FILE LAST UPDATED: 6 Feb 2002 (20020206/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

=> s780386/pn

S780386 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> s 780386/pn L1 0 780386/PN => s ep780386/pn L2 1 EP780386/PN

=> select 12 rn 1-E1 THROUGH E174 ASSIGNED

=> fil reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 4.01 4.16

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:55:16 ON 07 FEB 2002 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2002 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 5 FEB 2002 HIGHEST RN 389795-01-1 DICTIONARY FILE UPDATES: 5 FEB 2002 HIGHEST RN 389795-01-1

TSCA INFORMATION NOW CURRENT THROUGH July 7, 2001

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the H/Z/CA/CAplus files between 12/27/01 and 1/23/02. Use of the P indicator in online and SDI searches during this period, either directly appended to a CAS Registry Number or by qualifying an L-number with /P, may have yielded incomplete results. As of 1/23/02, the situation has been resolved. Also, note that searches conducted using the PREP role indicator were not affected.

Customers running searches and/or SDIs in the H/Z/CA/CAplus files incorporating CAS Registry Numbers with the P indicator between 12/27/01 and 1/23/02, are encouraged to re-run these strategies. Contact the CAS Help Desk at 1-800-848-6533 in North America or 1-614-447-3698, worldwide, or send an e-mail to help@cas.org for further assistance or to receive a credit for any duplicate searches.

=> s e1-e174 1 100-39-0/BI (100-39-0/RN) 1 101-55-3/BI (101-55-3/RN) 1 105-53-3/BI (105-53-3/RN) 1 111-44-4/BI

(111-44-4/RN)1 130312-01-5/BI (130312-01-5/RN) 1 13511-38-1/BI (13511-38-1/RN) 1 141907-41-7/BI (141907-41-7/RN) 1 142851-03-4/BI (142851-03-4/RN) 1 19099-93-5/BI (19099-93-5/RN) 1 193021-77-1/BI (193021-77-1/RN) 1 193021-78-2/BI (193021-78-2/RN) 1 193021-79-3/BI (193021-79-3/RN) 1 193021-80-6/BI (193021-80-6/RN) 1 193021-81-7/BI (193021-81-7/RN) 1 193021-82-8/BI (193021-82-8/RN) 1 193021-83-9/BI (193021-83-9/RN) 1 193021-84-0/BI (193021-84-0/RN) 1 193021-85-1/BI (193021-85-1/RN) 1 193021-86-2/BI (193021-86-2/RN) 1 193021-87-3/BI (193021-87-3/RN) 1 193021-88-4/BI (193021-88-4/RN) 1 193021-89-5/BI (193021-89-5/RN) 1 193021-90-8/BI (193021-90-8/RN) 1 193021-91-9/BI (193021-91-9/RN) 1 193021-92-0/BI (193021-92-0/RN) 1 193021-93-1/BI (193021-93-1/RN) 1 193021-94-2/BI (193021-94-2/RN) 1 193021-95-3/BI (193021-95-3/RN) 1 193021-96-4/BI (193021-96-4/RN) 1 193021-97-5/BI (193021-97-5/RN)

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1 6165-69-1/BI

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             1 637-69-4/BI
                 (637-69-4/RN)
             1 67-64-1/BI
                 (67-64-1/RN)
             1 6959-48-4/BI
                 (6959-48-4/RN)
             1 7051-34-5/BI
                 (7051-34-5/RN)
             1 84358-13-4/BI
                 (84358-13-4/RN)
             1 95798-23-5/BI
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             1 96835-17-5/BI
                 (96835-17-5/RN)
             1 98-80-6/BI
                 (98-80-6/RN)
L3
           174 (100-39-0/BI OR 101-55-3/BI OR 105-53-3/BI OR 111-44-4/BI OR
               130312-01-5/BI OR 13511-38-1/BI OR 141907-41-7/BI OR
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               193022-14-9/BI OR 193022-15-0/BI OR 193022-16-1/BI OR
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               2/BI OR 193022-18-3/BI OR 193022-19-4/BI OR 193022-20-7/BI OR
               193022-21-8/BI OR 193022-22-9/BI OR 193022-23-0/
=> d scan
                   REGISTRY COPYRIGHT 2002 ACS
L3
     174 ANSWERS
     Benzenethiol, 4-[(5-chloro-2-pyridinyl)oxy]- (9CI)
IN
MF
     C11 H8 C1 N O S
```

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):173

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidinecarboxamide,

N-(1,1-dimethylethoxy)-1-(methylsulfonyl)-4-[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI)

MF C24 H32 N2 O7 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Pentanamide, N-hydroxy-3-[(4-methoxyphenyl)sulfonyl]-2-methyl- (9CI)

MF C13 H19 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopentaneacetamide, N-hydroxy-1-[(4-phenoxyphenyl)sulfonyl]- (9CI)

MF C19 H21 N O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Piperidinecarboxylic acid, 4-hydroxy-, phenylmethyl ester (9CI)

MF C13 H17 N O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Piperidinecarboxylic acid, 4-[[(1,1-dimethylethoxy)amino]carbonyl]-4-[[(4-phenoxyphenyl)thio]methyl]-, 1,1-dimethylethyl ester (9CI)

MF C28 H38 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenebutanoic acid, .beta.-([1,1'-biphenyl]-4-ylsulfonyl)- (9CI)
MF C22 H20 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-acetamide, 4-[[4-(cyclohexyloxy)phenyl]sulfonyl]tetrahydro-Nhydroxy- (9CI)

MF C19 H27 N 06 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanamide, 3-[[4-(4-chlorophenoxy)phenyl]thio]-N-hydroxy-2,2-dimethyl(9CI)

MF C17 H18 C1 N O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopropane, (bromomethyl) - (7CI, 8CI, 9CI)

MF C4 H7 Br

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxylic acid, tetrahydro-4-(iodomethyl)-, ethyl ester (9CI)

MF C9 H15 I O3

Page 15

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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4-Piperidineacetamide, N-hydroxy-1-(2-methylpropyl)-4-[(4-IN phenoxyphenyl)sulfonyl]- (9CI)

MF C23 H30 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2002 ACS L3 174 ANSWERS

Cyclopentanecarboxamide, N-hydroxy-2-[(4-methoxyphenyl)sulfonyl]-, trans-IN (9CI)

C13 H17 N O5 S MF

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS 2H-Pyran-4-carboxamide, tetrahydro-N-hydroxy-4-[[[4-[4-(2-IN thienyl)phenoxy]phenyl]sulfonyl]methyl]- (9CI)

MF C23 H23 N O6 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-carboxylic acid, 4-[[[4-(4-bromophenoxy)phenyl]thio]methyl]tetr ahydro- (9CI)
MF C19 H19 Br O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzene, (bromomethyl) - (9CI)

MF C7 H7 Br

CI COM

 $Ph-CH_2-Br$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C17 H20 N2 O5 S

CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidineacetamide, N-(1,1-dimethylethoxy)-1-(1-methylethyl)-4-[(4-phenoxyphenyl)sulfonyl]-(9CI)

MF C26 H36 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanamide, N-hydroxy-.beta.-[(4-phenoxyphenyl)sulfonyl]- (9CI)

MF C22 H21 N O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopentaneacetamide, N-hydroxy-1-[(4-phenoxyphenyl)thio]- (9CI)

MF C19 H21 N O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Hydroxylamine, O-(1,1-dimethylethyl)-, hydrochloride (9CI)

MF C4 H11 N O . Cl H

 $H_2N-O-Bu-t$

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanoic acid, .beta.-[[4-(2-phenylethenyl)phenyl]sulfonyl]- (9CI)

MF C24 H22 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Piperidinecarboxamide,
4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl]-Nhydroxy-1-(methylsulfonyl)-, monohydrochloride (9CI)
MF C20 H23 C1 N2 O7 S2 . C1 H

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1-Piperidinecarboxylic acid, 4-[2-(hydroxyamino)-2-oxoethyl]-4-[(4-phenoxyphenyl)sulfonyl]-, phenylmethyl ester (9CI)
MF C27 H28 N2 O7 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C19 H19 Cl O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidinol (6CI, 7CI, 8CI, 9CI)

MF C5 H11 N O

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1,4-Piperidinedicarboxylic acid, 4-(hydroxymethyl)-,
1-(1,1-dimethylethyl)
4-ethyl ester (9CI)

MF C14 H25 N O5

$$\begin{array}{c|c} O & O \\ | & C - OBu - t \\ \hline \\ HO - CH_2 \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidineacetamide, N-hydroxy-1-(1-methylethyl)-4-[(4-phenoxyphenyl)sulfonyl]- (9CI)

MF C22 H28 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C16 H23 N O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl]tet
 rahydro-N-hydroxy-3-(phenylmethyl)- (9CI)
MF C26 H26 C1 N O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Acetic acid, (tetrahydro-4H-pyran-4-ylidene)- (9CI)
MF C7 H10 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenebutanoic acid, .beta.-[(4-bromophenyl)thio]- (9CI)
MF C16 H15 Br O2 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C17 H20 N2 O5 S . C1 H

Absolute stereochemistry.

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxylic acid, tetrahydro-4-[[[4-[4-(2-thienyl)phenoxy]phenyl]sulfonyl]methyl]- (9CI)

MF C23 H22 O6 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenepropanamide,
N-hydroxy-.alpha.-[[(4-methoxyphenyl)sulfonyl]methyl](9CI)
MF C17 H19 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-acetamide, N-(1,1-dimethylethoxy)tetrahydro-4-[(4-phenoxyphenyl)thio]- (9CI)

MF C23 H29 N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Piperidinecarboxylic acid, 4-oxo-, phenylmethyl ester (9CI)

MF C13 H15 N O3

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxylic acid, 4-(chloromethyl)tetrahydro-, ethyl ester
(9CI)
MF C9 H15 Cl O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C23 H27 C1 N2 O5 S

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Page 26

PROPERTY DATA AVAILABLE IN THE 'PROP', FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C20 H23 N O5 S

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Piperidinecarboxylic acid, 4-[[(1,1-dimethylethoxy)amino]carbonyl]-4[[(4-phenoxyphenyl)sulfonyl]methyl]-, 1,1-dimethylethyl ester (9CI)

MF C28 H38 N2 O7 S

Page 27

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanoic acid, 3-[[4-(4-chlorophenoxy)phenyl]thio]-2,2-dimethyl- (9CI) MF C17 H17 Cl O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Propanedioic acid, diethyl ester (9CI)
- MF C7 H12 O4
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C19 H25 N O4

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidinecarboxamide, 1-cyclopropyl-N-(1,1-dimethylethoxy)-4-[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI)

MF C26 H34 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanamide, N-hydroxy-.beta.-(2-naphthalenylsulfonyl)- (9CI)

MF C20 H19 N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopentaneacetamide, N-hydroxy-1-[(4-phenoxyphenyl)sulfinyl]- (9CI)

MF C19 H21 N O4 S

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS Benzenethiol, 4-(4-bromophenoxy)- (9CI) L3

IN

C12 H9 Br O S MF

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2002 ACS L3 174 ANSWERS

Propanamide, 2-[[(dimethylamino)sulfonyl]amino]-N-(1,1-dimethylethoxy)-3-ΙN [(4-phenoxyphenyl)sulfonyl]-, (R)- (9CI)

C21 H29 N3 O7 S2 MF

Absolute stereochemistry.

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Alaninamide, L-valyl-N-(1,1-dimethylethoxy)-3-[(4-phenoxyphenyl)sulfonyl]- (9CI)

MF C24 H33 N3 O6 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-[(5-chloro-2-pyridinyl)oxy]phenyl]sulfonyl]
methyl]tetrahydro-N-hydroxy- (9CI)
MF C18 H19 C1 N2 O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C19 H21 F N2 O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-(4-chlorophenoxy)phenyl]thio]methyl]tetrahy
dro-N-hydroxy- (9CI)
MF C19 H20 C1 N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN Boronic acid, 2-thienyl- (9CI)

MF C4 H5 B O2 S

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1,4-Piperidinedicarboxylic acid, 4-(hydroxymethyl)-,
1-(1,1-dimethylethyl)
ester (9CI)
MF C12 H21 N O5

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Piperidineacetamide, 1-(cyclopropylmethyl)-4-[[4-(4-fluorophenoxy)phenyl]sulfonyl]-N-hydroxy- (9CI)
MF C23 H27 F N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-acetamide, tetrahydro-N-hydroxy-

MF C19 H21 N O6 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-(4-bromophenoxy)phenyl]sulfonyl]methyl]tetr
ahydro-N-hydroxy- (9CI)
MF C19 H20 Br N O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 1,4-Piperidinedicarboxylic acid, 1-(1,1-dimethylethyl) 4-ethyl ester (9CI) MF C13 H23 N O4

REGISTRY COPYRIGHT 2002 ACS 174 ANSWERS L3 L-Alaninamide, ΙN ${\tt N-[(phenylmethoxy)\,carbonyl]-L-valyl-N-(1,1-dimethylethoxy)-}\\$ 3-[(4-phenoxyphenyl)sulfonyl]- (9CI) C32 H39 N3 O8 S MF

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
4-Piperidineacetamide, 1-(cyclopropylmethyl)-N-hydroxy-4-[(4-phenoxyhenyl)sulfonyl]- (9CI) L3 ΙN

C23 H28 N2 O5 S MF

Page 35

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxylic acid, tetrahydro-4-[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI)
MF C19 H20 O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenebutanamide, N-hydroxy-.beta.-[(4-methoxyphenyl)sulfonyl]- (9CI)
MF C17 H19 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide, N-(1,1-dimethylethoxy)tetrahydro-4-[[[4-(4-

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Carbamic acid, [(3S)-2-oxo-3-oxetanyl]-, phenylmethyl ester (9CI)

MF C11 H11 N O4

CI COM

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidineacetic acid, 4-[(4-phenoxyphenyl)thio]-1-

[(phenylmethoxy)carbonyl] - (9CI)

MF C27 H27 N O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN L-Cysteine, S-(4-phenoxyphenyl)-N-[(phenylmethoxy)carbonyl]- (9CI)

MF C23 H21 N O5 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Piperidinecarboxamide,
4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl]-Nhydroxy-, monohydrochloride (9CI)
MF C19 H21 C1 N2 O5 S . C1 H

HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-carboxamide, 4-[[[4-[(5-chloro-2-pyridinyl)oxy]phenyl]sulfonyl]

methyl]-N-(1,1-dimethylethoxy)tetrahydro- (9CI) MF C22 H27 C1 N2 O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-carboxylic acid, 4-[[[4-(4-chlorophenoxy)phenyl]thio]methyl]tet rahydro-, methyl ester (9CI) MF C20 H21 Cl O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Carbonochloridic acid, phenylmethyl ester (9CI)
- MF C8 H7 Cl O2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN Benzenethiol, 4-(4-pyridinyloxy)- (9CI)

C11 H9 N O S MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidinecarboxamide, N-(1,1-dimethylethoxy)-4-[[(4phenoxyphenyl)sulfonyl]methyl]-1-(3-pyridinylcarbonyl)- (9CI) C29 H33 N3 O6 S MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS Cyclopentanebutanamide, N-hydroxy-.beta.-[(4-methoxyphenyl)sulfonyl]-ΙN (9CI)

MF C16 H23 N O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-(4-chlorophenoxy)phenyl]sulfinyl]methyl]tet
rahydro-N-hydroxy- (9CI)
MF C19 H20 C1 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1,4-Piperidinedicarboxylic acid, 1-(1,1-dimethylethyl) ester (9CI)
MF C11 H19 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-acetic acid, tetrahydro-4-[(4-phenoxyphenyl)thio]- (9CI)
MF C19 H20 O4 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-carboxylic acid, 4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl letrahydro-, methyl ester (9CI) MF C20 H21 Cl O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Piperidinecarboxamide,
4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl]-Nhydroxy-1-(2-pyridinylmethyl)-, monohydrochloride (9CI)
MF C25 H26 C1 N3 O5 S . C1 H

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-acetamide,
4-[[4-(4-chlorophenoxy)phenyl]sulfonyl]tetrahydro-Nhydroxy- (9CI)
MF C19 H20 C1 N O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-(4-bromophenoxy)phenyl]thio]methyl]tetrahyd
ro-N-hydroxy- (9CI)
MF C19 H20 Br N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Pyridine, 3-(chloromethyl)-, hydrochloride (8CI, 9CI)
MF C6 H6 Cl N . Cl H

Page 43

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HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C12 H19 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C20 H24 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Thiopyran-4-acetamide, tetrahydro-N-hydroxy-4-[(4-phenoxyphenyl)sulfonyl]-, 1,1-dioxide (9CI)

MF C19 H21 N O7 S2

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxamide, tetrahydro-N-hydroxy-4-[[(4phenoxyphenyl)sulfonyl]methyl]- (9CI)

MF C19 H21 N O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-carboxylic acid, 4-[[[4-(4-chlorophenoxy)phenyl]thio]methyl]tet rahydro- (9CI)
MF C19 H19 C1 O4 S

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS L3

IN Boronic acid, phenyl- (9CI)

MF C6 H7 B O2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS L3

L-Alaninamide, L-valyl-N-hydroxy-3-[(4-phenoxyphenyl)sulfonyl]- (9CI) IN

C20 H25 N3 O6 S MF

COM CI

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS 4-Piperidinecarboxamide, N-(1,1-dimethylethoxy)-4-[[(4-IN

phenoxyphenyl) sulfonyl]methyl] - (9CI)

MF C23 H30 N2 O5 S

Page 46

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanamide, N-hydroxy-.beta.-(phenylsulfonyl)- (9CI)

MF C16 H17 N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanamide, 3-[[4-[(5-chloro-2-pyridinyl)oxy]phenyl]thio]-N-(1,1-dimethylethoxy)-2,2-dimethyl- (9CI)

MF C20 H25 C1 N2 O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenethiol, 4-phenoxy- (9CI)

MF C12 H10 O S

CI COM

Page 47

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanoic acid, .beta.-[[4-(phenylthio)phenyl]sulfonyl]- (9CI)

MF C22 H20 O4 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Carbamic acid, [2-[(1,1-dimethylethoxy)amino]-2-oxo-1-[[(4-phenoxyphenyl)sulfonyl]methyl]ethyl]-, phenylmethyl ester, (R)- (9CI)
MF C27 H30 N2 O7 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 4-Piperidinecarboxamide, 4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl]-N-

hydroxy-1-(3-pyridinylcarbonyl)-, monohydrochloride (9CI) MF C25 H24 C1 N3 O6 S . C1 H

● HCl

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS L3

4-Piperidineacetamide, N-hydroxy-4-[(4-phenoxyphenyl)sulfonyl]- (9CI) ΙN

C19 H22 N2 O5 S MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

REGISTRY COPYRIGHT 2002 ACS L3 174 ANSWERS

2H-Pyran-4-carboxylic acid,

4-[[[4-(4-bromophenoxy)phenyl]thio]methyl]tetr

ahydro-, ethyl ester (9CI) C21 H23 Br O4 S

MF

Page 49

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxylic acid, tetrahydro- (8CI, 9CI)

MF C6 H10 O3

CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C9 H16 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Piperidineacetic acid, 4-[2-(hydroxyamino)-2-oxoethyl]-4-[(4-

phenoxyphenyl)sulfonyl]-, ethyl ester (9CI)

MF C23 H28 N2 O7 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopentaneacetamide, N-hydroxy-1-[(4-methoxyphenyl)sulfonyl]- (9CI)

MF C14 H19 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxamide,

 $\hbox{\tt 4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl]} tet$

rahydro-N-hydroxy- (9CI)

MF C19 H20 C1 N 06 S

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS L3

2H-Pyran-4-carboxylic acid, tetrahydro-, ethyl ester (9CI) IN

MF C8 H14 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS L3

1,4-Dioxaspiro[4.5]decane-8-acetamide, N-hydroxy-8-[(4-ΙN phenoxyphenyl)sulfonyl]- (9CI) C22 H25 N O7 S

MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

2H-Pyran-4-carboxylic acid, IN

4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl

]tetrahydro-3-(phenylmethyl)- (9CI)

MF C26 H25 C1 O6 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-carboxylic acid, 4-[[[4-(4-bromophenoxy)phenyl]sulfonyl]methyl] tetrahydro- (9CI)
MF C19 H19 Br O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Piperidineacetamide, N-hydroxy-4-[(4-methoxyphenyl)sulfonyl]- (9CI)
MF C14 H20 N2 O5 S

$$\begin{array}{c|c} \text{MeO} & \text{O} & \text{NH} \\ \text{S} & \text{O} & \text{O} \\ \text{O} & \text{H} & \text{O} \\ \text{CH}_2-\text{C}-\text{NH}-\text{OH} \end{array}$$

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopentaneacetamide, N-(1,1-dimethylethoxy)-1-[(4-phenoxyphenyl)thio]-(9CI)

MF C23 H29 N O3 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanoic acid, 3-chloro-2,2-dimethyl- (9CI)

MF C5 H9 C1 O2

CI COM

$$\begin{array}{c} \text{Me} \\ \mid \\ \text{ClCH}_2-\text{C-CO}_2\text{H} \\ \mid \\ \text{Me} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxylic acid, 4-(bromomethyl)tetrahydro-, ethyl ester (9CI)

MF C9 H15 Br O3

REGISTRY COPYRIGHT 2002 ACS 174 ANSWERS L3 4-Piperidineacetamide, ΙN 1-(cyclopropylmethyl)-4-[(4-phenoxyphenyl)sulfonyl]-(9CI) C23 H28 N2 O4 S MF

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS Cyclohexanecarboxamide, N-hydroxy-2-[(4-methoxyphenyl)sulfonyl]-, trans-IN (9CI)

C14 H19 N O5 S MF

Relative stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxamide, tetrahydro-N-hydroxy-4-[[[4-[4-(3-

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-carboxylic acid, 4-[[[4-(4-fluorophenoxy)phenyl]thio]methyl]tet rahydro- (9CI)
MF C19 H19 F O4 S

- L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Benzene, 1-bromo-4-phenoxy- (9CI)
- MF C12 H9 Br O
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Propanamide, 2-[[(dimethylamino)sulfonyl]amino]-N-hydroxy-3-[(4-phenoxyphenyl)sulfonyl]-, (R)- (9CI)
- MF C17 H21 N3 07 S2
- CI COM

Absolute stereochemistry.

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidineacetamide, N-(1,1-dimethylethoxy)-1-methyl-4-[(4-phenoxyphenyl)sulfonyl]- (9CI)

MF C24 H32 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanamide, .beta.-([1,1'-biphenyl]-4-ylsulfonyl)-N-hydroxy- (9CI)

MF C22 H21 N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-acetamide, 4-[[4-(4-fluorophenoxy)phenyl]thio]tetrahydro-Nhydroxy- (9CI)

MF C19 H20 F N O4 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1-Piperidinecarboxylic acid, 4-(carboxymethylene)-, 1-(phenylmethylester)
(9CI)
MF C15 H17 N O4

O || C- O- CH₂- Ph |
N | CH- CO₂H

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Propanamide, 2-amino-N-hydroxy-3-[(4-phenoxyphenyl)sulfonyl]-, (2R)(9CI)
MF C15 H16 N2 O5 S
CI COM

Absolute stereochemistry.

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS L3

ΙN Propanamide, 2-amino-N-hydroxy-3-[(4-phenoxyphenyl)sulfonyl]-, monohydrochloride, (2R) - (9CI)

C15 H16 N2 O5 S . C1 H MF

Absolute stereochemistry.

● HCl

L3

174 ANSWERS REGISTRY COPYRIGHT 2002 ACS 2H-Pyran-4-carboxamide, tetrahydro-N-hydroxy-4-[[[4-(4-IN pyridinyloxy)phenyl]sulfonyl]methyl]-, monohydrochloride (9CI)

MFC18 H20 N2 O6 S . Cl H

HC1

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IN 1-Piperidinecarboxylic acid, 4-[2-(hydroxyamino)-2-oxoethyl]-4-[(4methoxyphenyl)sulfonyl]-, phenylmethyl ester (9CI)

MF C22 H26 N2 O7 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxylic acid, tetrahydro-4-[[[4-(4pyridinyloxy)phenyl]thio]methyl]- (9CI)

MF C18 H19 N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4H-Pyran-4,4-dicarboxylic acid, tetrahydro-, diethyl ester (6CI, 7CI, 8CI,

9CI)

MF C11 H18 O5

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxylic acid, tetrahydro-4-(hydroxymethyl)- (9CI)

MF C7 H12 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidineacetamide, N-hydroxy-4-[(4-phenoxyphenyl)sulfonyl]-1-(3pyridinylmethyl)- (9CI)

MF C25 H27 N3 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclohexaneacetamide, N-hydroxy-1-[(4-phenoxyphenyl)sulfonyl]- (9CI)

MF C20 H23 N O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-(4-fluorophenoxy)phenyl]sulfonyl]methyl]tet
rahydro-N-hydroxy- (9CI)
MF C19 H20 F N O6 S

- L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN Proteinase, matrix metallo- (9CI)
- MF Unspecified
- CI MAN
- *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
- L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
- IN 1-Piperidineacetic acid, 4-[2-[(1,1-dimethylethoxy)amino]-2-oxoethyl]-4[(4-phenoxyphenyl)sulfonyl]-, ethyl ester (9CI)
- MF C27 H36 N2 07 S

Page 63

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanamide, 2-[[(dimethylamino)sulfonyl]amino]-N-hydroxy-3-[(4-phenoxyphenyl)sulfonyl]-, monohydrochloride, (R)- (9CI)
MF C17 H21 N3 O7 S2 . C1 H

Absolute stereochemistry.

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxylic acid, tetrahydro-4-[[[4-[4-(3-thienyl)phenoxy]phenyl]sulfonyl]methyl]- (9CI)

MF C23 H22 O6 S2

PAGE 1-A

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanamide, N-hydroxy-.beta.-[(3-methoxyphenyl)sulfonyl]- (9CI)

MF C17 H19 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 3-Pyridinecarbonyl chloride, hydrochloride (9CI)
MF C6 H4 Cl N O . Cl H

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4-Piperidineacetamide,
1-acetyl-4-[[4-(4-fluorophenoxy)phenyl]sulfonyl]-Nhydroxy- (9CI)
MF C21 H23 F N2 O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Cyclohexaneacetamide, N-hydroxy-4-oxo-1-[(4-phenoxyphenyl)sulfonyl](9CI)
MF C20 H21 N O6 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2H-Pyran-4-carboxamide, N-(1,1-dimethylethoxy)tetrahydro-4-[[[4-(4-pyridinyloxy)phenyl]sulfonyl]methyl]- (9CI)

MF C22 H28 N2 O6 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 1,4-Piperidinedicarboxylic acid, 4-[[[4-(4-chlorophenoxy)phenyl]thio]methy

1]-, 1-(1,1-dimethylethyl) ester (9CI)

MF C24 H28 C1 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Ethane, 1,1'-oxybis[2-chloro- (9CI)

MF C4 H8 C12 O

CI COM

 $C1CH_2 - CH_2 - O - CH_2 - CH_2C1$

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenethiol, 4-(4-fluorophenoxy)- (9CI)

MF C12 H9 F O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidinecarboxamide, N-(1,1-dimethylethoxy)-4-[[(4phenoxyphenyl)sulfonyl]methyl]-1-(3-pyridinylmethyl)- (9CI)

MF C29 H35 N3 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanamide, N-hydroxy-.beta.-[[4-[2-(4-

methoxyphenyl)ethenyl]phenyl]sulfonyl]- (9CI)

MF C25 H25 N O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN 2H-Pyran-4-acetamide,

4-[[4-(4-fluorophenoxy)phenyl]sulfinyl]tetrahydro-Nhydroxy- (9CI)

MF C19 H20 F N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenethiol, 4-(4-chlorophenoxy)- (9CI)

MF C12 H9 Cl O S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopentaneacetic acid, 1-[(4-phenoxyphenyl)thio]- (9CI)

MF C19 H20 O3 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Alaninamide, L-valyl-N-hydroxy-3-[(4-phenoxyphenyl)sulfonyl]-,

monohydrochloride (9CI) MF C20 H25 N3 O6 S . Cl H

Absolute stereochemistry.

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanamide, 3-[[4-[(5-chloro-2-pyridinyl)oxy]phenyl]sulfonyl]-N-hydroxy-2,2-dimethyl-(9CI)

MF C16 H17 C1 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidineacetamide, 4-[[4-(4-chlorophenoxy)phenyl]sulfonyl]-N-hydroxy(9CI)

MF C19 H21 C1 N2 O5 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-(4-fluorophenoxy)phenyl]thio]methyl]tetrahy
dro-N-hydroxy- (9CI)
MF C19 H20 F N O4 S

$$S-CH_2$$
 $C-NH-OH$
 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS IN Boronic acid, 3-thienyl- (9CI) MF C4 H5 B O2 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2,7-Dioxaspiro[3.5]nonan-1-one (9CI)
MF C7 H10 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C21 H26 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-acetamide,
4-[[4-(4-fluorophenoxy)phenyl]sulfonyl]tetrahydro-Nhydroxy- (9CI)
MF C19 H20 F N O6 S

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanamide, 3-[[4-(4-chlorophenoxy)phenyl]sulfonyl]-N-hydroxy-2,2dimethyl- (9CI)

MF C17 H18 C1 N O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidineacetic acid, 4-[(4-phenoxyphenyl)thio]-, hydrochloride (9CI)

MF C19 H21 N O3 S . Cl H

● HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Propanone (9CI)

MF C3 H6 O

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-valyl-N-hydroxy-3-[(4-phenoxyphenyl)sulfonyl]- (9CI)

MF C28 H31 N3 O8 S

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Benzenebutanamide,
N-hydroxy-.beta.-[[4-(2-phenylethenyl)phenyl]sulfonyl](9CI)
MF C24 H23 N O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C22 H21 N O4 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxamide,
4-[[[4-[(5-chloro-2-pyridinyl)oxy]phenyl]thio]meth
yl]-N-(1,1-dimethylethoxy)tetrahydro- (9CI)
MF C22 H27 C1 N2 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 4H-Pyran-4-one, tetrahydro- (6CI, 7CI, 8CI, 9CI)

MF C5 H8 O2

CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzenebutanoic acid, .beta.-[(4-bromophenyl)sulfonyl]- (9CI)

MF C16 H15 Br O4 S

Page 76

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 4-Piperidinecarboxamide,

4-[[[4-(4-chlorophenoxy)phenyl]sulfonyl]methyl]-1-

(cyclopropylmethyl)-N-hydroxy-, monohydrochloride (9CI)

MF C23 H27 C1 N2 O5 S . C1 H

Page 77

Print selected from Online session

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

HCl

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Propanamide, 3-[[4-[(5-chloro-2-pyridinyl)oxy]phenyl]sulfonyl]-N-(1,1-dimethylethoxy)-2,2-dimethyl- (9CI)

MF C20 H25 C1 N2 O5 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2H-Pyran-4-carboxylic acid,
4-[[[4-(4-chlorophenoxy)phenyl]thio]methyl]tet
 rahydro-, ethyl ester (9CI)
MF C21 H23 C1 O4 S

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 174 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Print selected from Online session

Page 78

IN Benzene, 1-ethenyl-4-methoxy- (9CI)

MF C9 H10 O

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

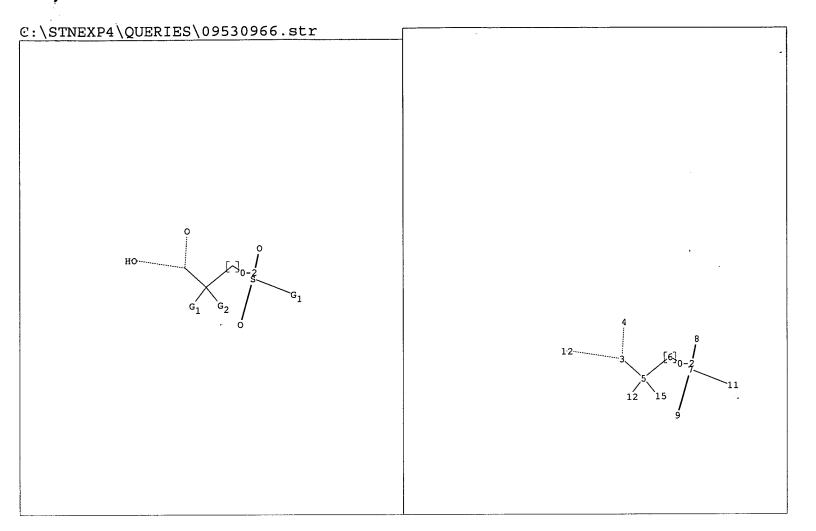
ALL ANSWERS HAVE BEEN SCANNED

=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y
COST IN U.S. DOLLARS
SINCE FILE

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 2.24 6.40

STN INTERNATIONAL LOGOFF AT 10:59:34 ON 07 FEB 2002



chain nodes :

1 2 3 4 5 6 7 8 9 11 12 15

chain bonds :

1-2 2-3 3-5 3-4 5-6 5-12 5-15 6-7 7-8 7-9 7-11

exact/norm bonds :

2-3 3-4 5-12 5-15 6-7 7-8 7-9 7-11

exact bonds :

1-2 3-5 5-6

G1:Cy,Ak

G2:0,N,X

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

9:CLASS 11:CLASS 12:CLASS 15:CLASS



ANSWER 1 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:72030 CAPLUS

DOCUMENT NUMBER: 136:134761

TITLE: Preparation of 3-arylsulfonyl-2-hydroxy-2-

methylpropanoic acids as inhibitors of matrix

metallo-proteinases (MMPs)

INVENTOR(S): Mantegani, Sergio; Bissolino, Pierluigi; Abrate,

Francesca; Cremonesi, Paolo; Perrone, Ettore

PATENT ASSIGNEE(S): Pharmacia + Upjohn S.p.A., Italy

SOURCE:

PCT Int. Appl., 50 pp. CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

Ι

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO. KI					ND	DATE			Α	PPLI	CATI	ои ис	ο.	DATE					
										_										
	WO	2002006215			Α	1	20020124			W	O 20	01-E	P773	6	2001					
		W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,		
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	PL,	PT,		
			RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,		
			UZ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ΤJ,	TM				
		RW:	GH,	GM,	ΚE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	ΤZ,	UG,	ZW,	AT,	BE,	CH,	CY,		
			DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,	TR,	BF,		
			ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	ΤG				
PRIORITY APPLN. INFO.:									(GB 2	000-	1743	5	Α	2000	0714				
OTHER SOURCE(S):						MARPAT 136:134761														
GI																				

AB The title compds. [I; X = NHOH, OH; R1 = OPh, SPh, SHet, Hyd, CH2Hyd; Het = heterocyclic ring; Hyd = substituted hydantoin-3-yl ring; A = Ph, Het, condensed Ph ring; R2 = H, Me; or R2 represents a methylene bridge connecting the N atom to the ortho position of said A to form a 5-membered

lactam] or their salts which are inhibitors of matrix metallo-proteinases (MMPs) and are therefore useful in the prevention, control and treatment

of diseases in which MMPs are involved, were prepd. E.g., a multi-step synthesis of I [A = 4-ClC6H4; X = OH; R1 = (3,4,4-trimethylhydantoin-1y1)CH2; R2 = H] which showed Ki of 14.7 nM against MMP-2, was given. 391903-52-9P 391903-53-0P 391903-54-1P IT 391903-55-2P 391903-56-3P 391903-57-4P 391903-58-5P 391903-59-6P 391903-60-9P 391903-61-0P 391903-62-1P 391903-63-2P 391903-64-3P 391903-65-4P 391903-66-5P 391903-67-6P 391903-68-7P 391903-69-8P 391903-70-1P 391903-71-2P 391903-72-3P 391903-73-4P 391903-74-5P 391903-76-7P 391903-77-8P 391903-78-9P 391903-79-0P 391904-13-5P 391904-15-7P 391904-16-8P 391904-18-0P 391904-19-1P 391904-22-6P 391904-23-7P 391904-24-8P 391904-25-9P 391904-26-0P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 3-arylsulfonyl-2-hydroxy-2-methylpropanoic acids as inhibitors of matrix metallo-proteinases (MMPs)) 391903-52-9 CAPLUS RN 1-Imidazolidinebutanoic acid, .alpha.-[[[4-[(4-CN chlorobenzoyl)amino]phenyl]sulfonyl]methyl]-.alpha.-hydroxy-3,4,4trimethyl-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 391903-53-0 CAPLUS

CN

1-Imidazolidinebutanoic acid, .alpha.-[[[4-[(4-fluorobenzoyl)amino]phenyl]sulfonyl]methyl]-.alpha.-hydroxy-3,4,4-trimethyl-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 2-A

RN 391903-54-1 CAPLUS

CN 1-Imidazolidinebutanoic acid, .alpha.-hydroxy-.alpha.-[[[4-[(4-methoxybenzoyl)amino]phenyl]sulfonyl]methyl]-3,4,4-trimethyl-2,5-dioxo-(9CI) (CA INDEX NAME)

PAGE 2-A

RN 391903-55-2 CAPLUS
CN Propanoic acid,

3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]- (9CI) (CA INDEX NAME)

RN 391903-56-3 CAPLUS

CN Propanoic acid,

2-hydroxy-2-[[[4-[(4-methoxybenzoyl)amino]phenyl]sulfonyl] methyl]-3-(phenylthio)- (9CI) (CA INDEX NAME)

RN 391903-57-4 CAPLUS

CN Propanoic acid, 2-hydroxy-2-[(phenylthio)methyl]-3-[[4-[(4-pyridinylcarbonyl)amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & OH \\ \hline C-NH & O & OH \\ \hline S-CH_2-C-CH_2-SPh \\ \hline O & CO_2H \end{array}$$

Na

RN 391903-61-0 CAPLUS

CN Propanoic acid,

3-[[4-[(4-fluorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391903-62-1 CAPLUS

CN Propanoic acid,

3-[[4-[(4-cyanobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391903-63-2 CAPLUS

CN Propanoic acid, 2-hydroxy-2-(phenoxymethyl)-3-[[4-[(4-pyridinylcarbonyl)amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 391903-64-3 CAPLUS

CN Propanoic acid,

3-[[4-[(4-bromobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391903-65-4 CAPLUS

CN Propanoic acid,

3-[[4-[[4-(dimethylamino)benzoyl]amino]phenyl]sulfonyl]-2hydroxy-2-(phenoxymethyl)-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 391903-66-5 CAPLUS

CN Propanoic acid,

2-hydroxy-2-[[[4-[(4-methoxybenzoyl)amino]phenyl]sulfonyl] methyl]-3-phenoxy- (9CI) (CA INDEX NAME)

RN 391903-67-6 CAPLUS

CN Propanoic acid,

3-[[4-[(1,3-benzodioxol-5-ylcarbonyl)amino]phenyl]sulfonyl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391903-68-7 CAPLUS

CN Propanoic acid, 3-[[4-(benzoylamino)phenyl]sulfonyl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391903-69-8 CAPLUS

CN Propanoic acid,

3-[[4-(1,3-dihydro-1-oxo-2H-isoindol-2-yl)phenyl]sulfonyl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391903-70-1 CAPLUS

CN Propanoic acid, 3-[[4-[(4-chlorobenzoyl)methylamino]phenyl]sulfonyl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391903-71-2 CAPLUS

CN Propanoic acid,

3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[(2-thiazolylthio)methyl]- (9CI) (CA INDEX NAME)

RN 391903-72-3 CAPLUS

CN Propanoic acid,

3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[(2-pyridinylthio)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CO_2H \\ \parallel & \parallel \\ C-NH & O & OH \\ \end{array}$$

RN 391903-73-4 CAPLUS

CN Propanoic acid,

3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[[(4-hydroxyphenyl)thio]methyl]- (9CI) (CA INDEX NAME)

RN 391903-74-5 CAPLUS

CN Propanoic acid, 3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-[[(4-fluorophenyl)thio]methyl]-2-hydroxy- (9CI) (CA INDEX NAME)

RN 391903-76-7 CAPLUS

CN 1-Imidazolidinepropanoic acid, .alpha.-[[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]methyl]-.alpha.-hydroxy-3,4,4-trimethyl-2,5-dioxo- (9CI) (CA INDEX NAME)

Page 150

09530965.trn

PAGE 2-A

RN 391903-77-8 CAPLUS

CN Propanoic acid, 2-hydroxy-2-(phenoxymethyl)-3-[[4-[[4-(trifluoromethoxy)benzoyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 391903-78-9 CAPLUS

CN Propanoic acid, 2-hydroxy-2-(phenoxymethyl)-3-[[4-[[4-(trifluoromethyl)benzoyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 391903-79-0 CAPLUS

CN Propanoic acid,

3-[[4-[(4-fluorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[[(4-hydroxyphenyl)thio]methyl]- (9CI) (CA INDEX NAME)

Hong Liu

RN 391904-15-7 CAPLUS

CN Propanoic acid,

3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 391904-16-8 CAPLUS

CN Propanoic acid,

3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[(2-thiazolylthio)methyl]-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 391904-18-0 CAPLUS

CN Propanoic acid,

3-[[4-[(4-chlorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[(2-pyridinylthio)methyl]-, monosodium salt (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O & CO_2H \\
 & S - CH_2 - C - CH_2 - S \\
 & O & OH \\
\end{array}$$

Na

RN 391904-19-1 CAPLUS

CN Propanoic acid,

3-[[4-[(4-fluorobenzoyl)amino]phenyl]sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]- (9CI) (CA INDEX NAME)

RN 391904-22-6 CAPLUS

CN Propanoic acid, 2-hydroxy-2-(phenoxymethyl)-3-[[4-[[4-(1-pyrrolidinyl)benzoyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 391904-23-7 CAPLUS

CN Propanoic acid,

3-[[4-[[(6-chloro-3-pyridinyl)carbonyl]amino]phenyl]sulfon yl]-2-hydroxy-2-(phenoxymethyl)- (9CI) (CA INDEX NAME)

RN 391904-24-8 CAPLUS

CN Propanoic acid, 2-hydroxy-2-[(phenylthio)methyl]-3-[[4-[(4-propoxybenzoyl)amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 391904-25-9 CAPLUS

Page 154 09530965.trn

CN Propanoic acid, 2-hydroxy-2-[(phenylthio)methyl]-3-[[4-[[4-(trifluoromethoxy)benzoyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

391904-26-0 CAPLUS RN

Propanoic acid, 2-hydroxy-2-[(phenylthio)methyl]-3-[[4-[[4-CN (trifluoromethyl)benzoyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 2 OF 19 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 2001:746581 CAPLUS

2

DOCUMENT NUMBER:

136:167154

TITLE:

.alpha.-Alkyl-.alpha.-amino-.beta.-sulfone

hydroxamates as potent MMP inhibitors that spare

MMP-1

AUTHOR(S):

Becker, D. P.; DeCrescenzo, G.; Freskos, J.; Getman, D. P.; Hockerman, S. L.; Li, M.; Mehta, P.; Munie, G.

E.; Swearingen, C.

CORPORATE SOURCE:

Departments of Medicinal Chemistry and Inflammation-Oncology, Pharmacia Research &

Development, Skokie, IL, 60077, USA

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2001),

11(20), 2723-2725

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier Science Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE: English

A series of .alpha.-alkyl-.alpha.-amino-.beta.-sulfonyl hydroxamates HONHCOCR1(NR2R3)CH2SO2C6H4XPh-4 [R1 = Me, R2 = H, Ac, Me, Et, CH2Ph, CH2CH2Ph, 3,4-methylenedioxybenzyl, 2-naphthylmethyl, propargyl,

pyrrolidinoacetyl, R3 = H, X = 0; R1-R3 = Me, X = 0; R1 = Me, R2 = H, Ac,

R3 = H, X = S; R1 = Ph, R2 = Bz, H, R3 = H, X = O; R1R2 = (CH2)3, R3 = propargyl, X = O] was prepd. and evaluated for potency vs. MMP-2 and MMP-13, and for selectivity vs. MMP-1. Low nanomolar potency was obtained

with selectivity vs. MMP-1 ranging from >10 to >1000. Selected compds. were orally bioavailable.

IT 397330-26-6P 397330-28-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(.alpha.-alkyl-.alpha.-amino-.beta.-sulfonyl hydroxamates as potent

MMP

inhibitors that spare MMP-1)

RN 397330-26-6 CAPLUS

CN Alanine, 2-[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

RN 397330-28-8 CAPLUS

CN Alanine, N-acetyl-2-[[[4-(phenylthio)phenyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ACCESSION NUMBER: 2001:730698 CAPLUS

9

DOCUMENT NUMBER: 135:289056

TITLE: Preparation of amidino compounds useful as nitric

oxide synthase inhibitors

INVENTOR(S): Webber, Ronald Keith; Awasthi, Alok K.; Bergmanis,

Arija A.; Durley, Richard C.; Ganser, Scott S.;

Hagen,

Timothy J.; Hallinan, Ann E.; Hansen, Donald W.; Hickory, Brian S.; Moormann, Alan E.; Pitzele,

Barnett

S.; Promo, Michelle A.; Schartman, Richard R.;

Snyder,

Jeffrey S.; Trivedi, Mahima; Tsymbalov, Sofya

PATENT ASSIGNEE(S): Pharmacia Corporation, USA SOURCE: PCT Int. Appl., 144 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

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APPLICATION NO. DATE
    PATENT NO.
                    KIND DATE
    WO 2001072703 A1 20011004 WO 2001-US9433 20010323
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
            HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
            LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
            RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ,
            VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
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            DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                         US 2001-816577 20010323
                     A1 20020214
    US 2002019563
                                       US 2000-191923P P 20000324
PRIORITY APPLN. INFO.:
                        MARPAT 135:289056
OTHER SOURCE(S):
    The invention relates to S-[2-[(1-iminoethyl)amino]ethyl]-2-methyl-L-
    cysteine (1) or its pharmaceutically acceptable salts for use as nitric
    oxide synthase (NOS) inhibitors. Thus, 1.2HCl was prepd. by a multistep
    procedure involving S-alkylation of (2R)-2-methyl-L-cysteine
hydrochloride
    with Boc-NHCH2CH2Br (Boc = tert-butoxycarbonyl), deprotection,
     condensation with Et acetimidate hydrochloride, and acidolysis with 1 N
    HCl. (2R)-2-methyl-L-cysteine hydrochloride was obtained from
     (R)-cysteine Me ester hydrochloride. Inhibitory assays for compd. 1.2HCl
    showed hiNOS, hecNOS, hncNOS, and human cartilage IC50 values 3.1, 77, 15
     .mu.M, and 0.7 .mu.M, resp.
     364067-25-4P
    RL: BAC (Biological activity or effector, except adverse); BSU
(Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of amidino compds. useful as nitric oxide synthase inhibitors)
RN
     364067-25-4 CAPLUS
    L-Alanine, 3-[[2-[(1-iminoethyl)amino]ethyl]sulfonyl]-2-methyl-,
CN
    dihydrochloride (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

●2 HCl

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

/D6 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:730697 CAPLUS

DOCUMENT NUMBER: 135:273215

TITLE: Preparation of amidino compounds useful as nitric

oxide synthase inhibitors

INVENTOR(S): Webber, Ronald Keith; Awasthi, Alok K.; Bergmanis,

Arija A.; Durley, Richard C.; Fok, Kam F.; Ganser,

Scott S.; Hagen, Timothy J.; Hallinan, Ann E.;

Hansen,

Donald W.; Hickory, Brian S.; Manning, Pamela T.;

Mao,

Michael; Moormann, Alan E.; Pitzele, Barnett S.; Promo, Michelle A.; Schartman, Richard R.; Scholten, Jeffrey A.; Snyder, Jeffrey S.; Toth, Mihaly V.; Trivedi, Mahima; Tsymbalov, Sofya; Tjoeng, Foe Siong

PATENT ASSIGNEE(S): Pharmacia Corporation, USA

SOURCE:

PCT Int. Appl., 159 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE: E FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT	PATENT NO.							A	PPLI	CATI	и ис	٥.	DATE			
WO 200	0 2001072702			2	2001	1004		W	0323							
W:	W: AE, AG,			AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,
	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,	LS,
	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,
	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	ŪG,	US,	UZ,
	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM			
RW	: GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,
	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG		
US 200								US 2001-816577 20010323								
PRIORITY AP	PLN.	INFO	. :				1	US 2000-191923P P 20000324								
OTHER SOURC	E(S):			MAR	PAT	135:	2732	15								
AB Amidin	o com	pds.	R11	N:CR	13NR	12CR	9R10	CR1R	7-X-	CR5R	6CR2	(NR3	3R4)C	OR8	[X =	s,

SO2; R1, R5, R6, R7 = H, halo, alkyl (alkyl and other groups may be substituted), alkenyl, alkynyl, alkoxyalkyl; R2 = alkyl, alkenyl, alkynyl,

alkoxyalkyl, alkylthioalkyl; R3 = H, OH, CHO, alkanoyl, CO2H, C(O)SH or alkyl esters; R8 = OH, alkoxy, an amino or alkylamino group or R3 and R8 may form a ring; R4 = H, CO2H, carbalkoxy; R9, R10 = H, alkyl, alkenyl, alkynyl, alkoxyalkyl; R11, R12 = H, OH, CO2H, C(O)SH or esters or R11 and R12 may form a ring; R13 = alkyl (with provisos)] or their salts were prepd. as nitric oxide synthase (NOS) inhibitors. Thus, S-[2-[(1-iminoethyl)amino]ethyl]-2-methyl-L-cysteine dihydrochloride (1) was prepd. by a multistep procedure involving S-alkylation of (2R)-2-methyl-L-cysteine hydrochloride with Boc-NHCH2CH2Br (Boc = tert-butoxycarbonyl), deprotection, condensation with Et acetimidate hydrochloride, and acidolysis with 1 N HCl. (2R)-2-methyl-L-cysteine hydrochloride was obtained from (R)-cysteine Me ester hydrochloride. Inhibitory assays for compd. 1 showed hiNOS, hecNOS, hncNOS, and human cartilage IC50 values 3.1, 77, 15 .mu.M, and 0.7 .mu.M, resp.

364067-25-4P 364068-52-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of amidino compds. useful as nitric oxide synthase inhibitors)

RN 364067-25-4 CAPLUS

L-Alanine, 3-[[2-[(1-iminoethyl)amino]ethyl]sulfonyl]-2-methyl-, CN dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● 2 HCl

RN 364068-52-0 CAPLUS

L-Alanine, 3-[[2-[(1-iminoethyl)amino]ethyl]sulfonyl]-2-methyl- (9CI) CN

(CA

INDEX NAME)

Absolute stereochemistry.

Page 159 09530965.trn

ANSWER 5 OF 19 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 2001:396841 CAPLUS

DOCUMENT NUMBER: 135:5449

Preparation of (R)-3-(4-chlorobiphenylsulfonyl)-2-TITLE:

hydroxy-2-(phenylthio)methylpropionic acid and its

use

as a matrix metalloproteinase inhibitor in the

treatment of cancer

Bissolino, Pierluigi; Mantegani, Sergio; Orzi, INVENTOR(S):

Fabrizio; Jabes, Daniela; Alzani, Rachele; D'anello,

Matteo; Perrone, Ettore

PATENT ASSIGNEE(S):

Pharmacia + Upjohn S.P.A., Italy

SOURCE:

PCT Int. Appl., 25 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

F	PATENT NO.					DATE		APPLICATION NO. DATE											
-																			
N.	0 2001	2001038301			A1 20010531			WO 2000-EP10837 20001101											
	W:	ΑE,	AG,	AL,	ΑM,	AT,	ΑU,	ΑZ,	ΒA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
		CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,		
		HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,		
		LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	PL,	PT,	RO,	RU,		
		SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	ΤZ,	UA,	UG,	US,	UZ,	VN,		
		YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM						
	RW:	GH,	GM,	ΚE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	ΤZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,		
		DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,	TR,	BF,		
		ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG				
PRIORI	TY APP	LN.	INFO	.:				GB 1999-27453 A 19991119											
OTHER	SOURCE	(S):			CAS	REAC'	г 13	5:54	49										
AB ((R) - 3 - (4-ch	loro	biph	enyl	sulf	onyl) -2-1	hydr	oxy-	2-(p)	heny.	lthi	o)me	thyl	prop.	ionic		
а	cid an	d it	s sa	lts,	use	ful a	as a	mat:	rix ı	meta.	llop	rote	inas	e inl	nibii	tor :	in the		
t	reatme	nt o	f car	ncer	s, i	s pr	epd.	alo	ng w	ith:	its	salt	s.						

the 226419-98-3P 341498-84-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in the prepn. of (R)-3-(4-chlorobiphenylsulfonyl)-2-hydroxy-2-(phenylthio)methylpropionic acid and its salts as matrix metalloproteinase inhibitors useful in the treatment of cancers)

RN 226419-98-3 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl] - (9CI) (CA INDEX NAME)

RN 341498-84-8 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]-, (2R)-, compd. with (.alpha.S)-.alpha.-[(1R)-1-(methylamino)ethyl]benzenemethanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 341498-83-7 CMF C22 H19 C1 O5 S2

Absolute stereochemistry. Rotation (+).

CM 2

CRN 321-98-2 CMF C10 H15 N O

Absolute stereochemistry. Rotation (+).

IT 341498-83-7P 341498-89-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of (R)-3-(4-chlorobiphenylsulfonyl)-2-hydroxy-2-(phenylthio) methylpropionic acid and its salts as matrix

metalloproteinase inhibitors useful in the treatment of cancers)

RN 341498-83-7 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 341498-89-3 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Na

IT 341498-92-8P 341498-95-1P 341498-98-4P 341499-01-2P 341499-04-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological $\,$

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of (R)-3-(4-chlorobiphenylsulfonyl)-2-hydroxy-2-(phenylthio)methylpropionic acid and its salts as matrix

metalloproteinase inhibitors useful in the treatment of cancers)

RN 341498-92-8 CAPLUS

CN L-Arginine, mono[(2R)-3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]propanoate] (9CI) (CA INDEX NAME)

CM 1

CRN 341498-83-7 CMF C22 H19 C1 O5 S2

Absolute stereochemistry. Rotation (+).

CM 2

CRN 74-79-3 CMF C6 H14 N4 O2 CDES 5:L

Absolute stereochemistry.

$$H_2N$$
 N_H
 $(CH_2)_3$
 S
 CO_2H
 N_H

CM 1

CRN 341498-83-7 CMF C22 H19 C1 O5 S2

Absolute stereochemistry. Rotation (+).

CM 2

CRN 6284-40-8 CMF C7 H17 N O5 CDES *

Absolute stereochemistry.

RN 341498-98-4 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]-, monopotassium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

K

RN 341499-01-2 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]-, calcium salt (2:1), (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●1/2 Ca

RN 341499-04-5 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]-, magnesium salt (2:1), (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●1/2 Mg

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L5 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1999:354468 CAPLUS

2

Page 165 09530965.trn

DOCUMENT NUMBER:

131:18833

TITLE:

Preparation of .alpha.-hydroxy, -amino, and halo derivatives of .beta.-sulfonyl hydroxamic acids as

matrix metalloproteinases inhibitors

INVENTOR(S):

Warpehoski, Martha A.; Mitchell, Mark Allen; Harper,

Donald E.; Maggiora, Linda Louise

PATENT ASSIGNEE(S):

Pharmacia & Upjohn Company, USA PCT Int. Appl., 46 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

		CENT				ND	DATE			Ï		CATI			DATE			
	WO	9926	909		A		19990603 19990826			7	1118							
		W:										BY,						
												HR, LU,						
												SG,						
												AZ,						
TM		RW: GH, GM,		KE	T.S	М₩	SD.	S.7.	UG	. 7.W.	ΔТ.	BE.	CH.	CY.	DE.	DK.	ES.	
		1/1/										PT,						
							ML,											
							19990615 20000927											
	EF											IT,					MC,	PT,
							FI,		·									
		9814																
	JP 2001524462 T2 NO 2000002505 A																	
PRIORITY APPLN. INFO.:												.7265						
												IB21						
OTHER SOURCE(S): MARPAT 131:18833																		

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GI

The title compds. [I; R1 = C4-12 alkyl, C4-12 alkenyl, C4-12 alkynyl, AB etc.; R2 = C1-12 alkyl, C4-12 alkenyl, C4-12 alkynyl, etc.; Y = OH, NR9R10, F; R9, R10 = H, COR3, CO2R3, etc.; R3 = H, cycloalkyl, alkyl, etc.], inhibitors of matrix metalloproteinases which are useful in treating osteoarthritis, rheumatoid arthritis, septic arthritis, osteoporosis, tumor metastasis, periodontitis, gingivitis, corneal ulceration, dermal ulceration, gastric ulceration, inflammation, or

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asthma, were prepd. E.g., a 7-step synthesis of I [R1 = 4-PhC6H4; R2 =
     4-MeOC6H4SO2CH2; Y = OH] which showed Ki of 0.074 .mu.M and 0.0019 .mu.M
     against stromelysin and gelatinase, resp.
     226419-90-5P 226419-91-6P 226419-92-7P
IT
     226419-93-8P 226419-94-9P 226419-95-0P
     226419-96-1P 226419-97-2P 226419-98-3P
     226419-99-4P 226420-00-4P 226420-01-5P
     226420-02-6P 226420-03-7P 226420-04-8P
     226420-05-9P 226420-06-0P 226420-07-1P
     226420-08-2P 226420-09-3P 226420-10-6P
     226420-11-7P 226420-12-8P 226420-13-9P
     RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); USES (Uses)
        (prepn. of .alpha.-hydroxy, -amino, and halo derivs. of
.beta.-sulfonyl
        hydroxamic acids as matrix metalloproteinases inhibitors)
     226419-90-5 CAPLUS
RN
     1-Imidazolidinepropanoic acid,
.alpha.-[[(4-butoxyphenyl)sulfonyl]methyl]-
     3-butyl-.alpha.-hydroxy-2,5-dioxo- (9CI) (CA INDEX NAME)
 n-Bu
     CH<sub>2</sub>
 HO-C-CO2H
     CH<sub>2</sub>
     OBu-n
RN
     226419-91-6 CAPLUS
'CN
     1-Imidazolidinepropanoic acid,
.alpha.-[[(4-butoxyphenyl)sulfonyl]methyl]-
     .alpha.-hydroxy-3,4,4-trimethyl-2,5-dioxo- (9CI) (CA INDEX NAME)
```

RN 226419-92-7 CAPLUS

CN Propanoic acid, 3-[(4-butoxyphenyl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]- (9CI) (CA INDEX NAME)

RN 226419-93-8 CAPLUS

CN Propanoic acid, 3-[(4-butoxyphenyl)sulfonyl]-2-hydroxy-2-[[(phenylmethyl)thio]methyl]- (9CI) (CA INDEX NAME)

RN 226419-94-9 CAPLUS

CN Pentonic acid, 2-C-[[(4-butoxyphenyl)sulfonyl]methyl]-3,5-dideoxy-4-S-(phenylmethyl)-4-thio-(9CI) (CA INDEX NAME)

RN 226419-95-0 CAPLUS

CN 1-Imidazolidinepropanoic acid, .alpha.-[[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]methyl]-.alpha.-hydroxy-3-methyl-2,5-dioxo-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 226419-96-1 CAPLUS

CN 1-Imidazolidinepropanoic acid, 3-butyl-.alpha.-[[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]methyl]-.alpha.-hydroxy-2,5-dioxo- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 226419-97-2 CAPLUS

CN 1-Imidazolidinepropanoic acid, .alpha.-[[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]methyl]-.alpha.-hydroxy-3,4,4-trimethyl-2,5-dioxo-(9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 226419-98-3 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[(phenylthio)methyl]- (9CI) (CA INDEX NAME)

RN 226419-99-4 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[[(phenylmethyl)thio]methyl]- (9CI) (CA INDEX NAME)

RN 226420-00-4 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2- [(2-pyridinylthio)methyl]- (9CI) (CA INDEX NAME)

RN 226420-01-5 CAPLUS

CN Propanoic acid, 3-[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]-2-hydroxy-2-[[[(5-methyl-3-isoxazolyl)methyl]thio]methyl]- (9CI) (CA INDEX NAME)

RN 226420-02-6 CAPLUS

CN Pentonic acid,

2-C-[[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]methyl]-3,4,5trideoxy-4-(3-methyl-2,5-dioxo-1-imidazolidinyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 226420-03-7 CAPLUS

CN Pentonic acid, 2-C-[[(4'-chloro[1,1'-biphenyl]-4-yl)sulfonyl]methyl]-3,5-dideoxy-4-S-(phenylmethyl)-4-thio- (9CI) (CA INDEX NAME)

RN 226420-04-8 CAPLUS
CN 1-Imidazolidinepropanoic acid,
.alpha.-hydroxy-3-methyl-2,5-dioxo-.alpha.[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

RN 226420-05-9 CAPLUS
CN 1-Imidazolidinepropanoic acid, 3-butyl-.alpha.-hydroxy-2,5-dioxo-.alpha.[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

RN 226420-06-0 CAPLUS

CN 1-Imidazolidinepropanoic acid, .alpha.-hydroxy-3,4,4-trimethyl-2,5-dioxo-.alpha.-[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

RN 226420-07-1 CAPLUS

CN Propanoic acid, 2-hydroxy-2-[[(4-phenoxyphenyl)sulfonyl]methyl]-3-(phenylthio)- (9CI) (CA INDEX NAME)

RN 226420-08-2 CAPLUS

CN Propanoic acid, 2-hydroxy-2-[[(4-phenoxyphenyl)sulfonyl]methyl]-3[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)

RN 226420-09-3 CAPLUS

CN Pentonic acid,

3,4,5-trideoxy-4-(3-methyl-2,5-dioxo-1-imidazolidinyl)-2-C[[(4-phenoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

RN 226420-10-6 CAPLUS

CN Pentonic acid, 3,5-dideoxy-4-S-(1-methyl-1H-imidazol-2-yl)-2-C-[[(4-phenoxyphenyl)sulfonyl]methyl]-4-thio-(9CI) (CA INDEX NAME)

RN 226420-11-7 CAPLUS

CN 1-Imidazolidinepropanoic acid, .alpha.-hydroxy-3,4,4-trimethyl-2,5-dioxo-.alpha.-[[[4-(4-pyridinyl)phenyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 226420-12-8 CAPLUS

CN Propanoic acid, 2-hydroxy-2-[(phenylthio)methyl]-3-[[4-(4-pyridinyl)phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 226420-13-9 CAPLUS

CN 1-Imidazolidinepropanoic acid, .alpha.-hydroxy-3,4,4-trimethyl-2,5-dioxo-.alpha.-[[[4-(4-pyridinyloxy)phenyl]sulfonyl]methyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

IT 226420-18-4P 226420-21-9P 226420-22-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of .alpha.-hydroxy, -amino, and halo derivs. of .beta.-sulfonyl

hydroxamic acids as matrix metalloproteinases inhibitors)

RN 226420-18-4 CAPLUS

CN Propanoic acid, 3-([1,1'-biphenyl]-4-ylsulfonyl)-2-hydroxy-2-[[(4-methoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

RN 226420-21-9 CAPLUS

CN Propanoic acid, 3-(benzoylamino)-2-hydroxy-2-[[(4-methoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

RN 226420-22-0 CAPLUS

CN Propanoic acid, 2-hydroxy-3-[(4-methoxybenzoy1)amino]-2-[[(4-methoxyphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1998:612095 CAPLUS

Page 179 09530965.trn

DOCUMENT NUMBER: 129:244921

TITLE: Preparation of aromatic sulfonyl alpha-hydroxy

hydroxamic acid compounds as matrix metalloprotease

inhibitors

Freskos, John N.; Boehm, Terri L.; Mischke, Brent V.; INVENTOR(S):

Heintz, Robert M.; Mcdonald, Joseph J.; Decrescenzo,

Gary A.; Howard, Susan C.

PATENT ASSIGNEE(S): Monsanto Company, USA PCT Int. Appl., 203 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.			KIND DATE					APPLICATION NO.					DATE				
	WO	WO 9839326			A1 19980911			WO 1998-US4277				19980304						
		W:	AL,	AU,	BA,	BB,	BG,	BR,	CA,	CN,	CU,	CZ,	EE,	GE,	GH,	GW,	HU,	ID,
			IL,	IS,	JP,	KP,	KR,	LC,	LK,	LR,	LT,	LV,	MG,	MK,	MN,	MX,	NO,	NZ,
			PL,	RO,	SG,	SI,	SK,	SL,	TR,	TT,	UA,	US,	UZ,	VN,	YU,	AM,	AZ,	BY,
			KG,	KZ,	MD,	RU,	ТJ,	TM		•	-	•	•		•	•	-	•
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	DE,	DK,	ES,	FI,
															CF,			
			GΑ,	GN,	ML,	MR,	NE,	SN,	TD,	TG								
	ΑU	9864	478		A	1	1998	0922		A	U 19	98-6	4478		1998	0304		
	ΑU	7373	29		B	2	2001	0816										
	ΕP	9849	59		A.	1	2000	0315		E	P 19	98-9	1017	7	19980	0304		
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	PT,	IE,
FΙ																		
	BR	9808	150		Α		2000	0328		В	R 19	98-8	150		19980	0304		
PRIO	RITY	APP.	LN.	INFO	.:					US 1	997-	3518	2 P	P	19970	0304		
											998-	US42	77	W	19980	0304		
OTHE:	R SC	URCE	(S):			MAR	PAT :	129:	2449	21								
ΔR	The.	1 + i + i	10 0	amad	e U	SHIP	(O) C	(OU)	/D21/	വാദ	02P1	ГТ.	D2 -	_ u	C1 - i	1 -11	2557	C1 - I

AΒ The title compds. HONHC(O)C(OH)(R2)CH2SO2R1 [I; R2 = H, C1-4 alkyl, C1-4haloalkyl, etc.; R1 = 5-6 membered cycloalkyl, heterocyclyl, aryl, etc.] which inter alia inhibit matrix metalloprotease activity, were prepd. Thus, multi-step synthesis of I [R1 = 4-PhOC6H4; R2 = Me] which showed 51.9% inhibition of angiogenesis in the cornea of a mouse, was described.

ΙT 213184-20-4P 213184-29-3P 213184-51-1P 213184-61-3P 213184-63-5P 213184-65-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of arom. sulfonyl alpha-hydroxy hydroxamic acid compds. as matrix metalloprotease inhibitors)

213184-20-4 CAPLUS RN

CN Propanoic acid, 2-hydroxy-2-methyl-3-[(4-phenoxyphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 213184-29-3 CAPLUS

CN Propanoic acid, 3-[[4-(3,4-dimethylphenoxy)phenyl]sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)

RN 213184-51-1 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[(4-nitrophenyl)sulfonyl]- (9CI)

(CA INDEX NAME)

RN 213184-61-3 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[[4-[[(2-methylphenyl)amino]carbonyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

RN 213184-63-5 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[[4-[[[(3-

Page 181 09530965.trn

methylphenyl)amino]carbonyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

213184-65-7 CAPLUS RN

Propanoic acid, 2-hydroxy-2-methyl-3-[[4-[[[(4-CN

methylphenyl)amino]carbonyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

ANSWER 8 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1995:532307 CAPLUS

DOCUMENT NUMBER:

122:278041

TITLE:

Photographic couplers having a ballast containing a

sulfone or sulfoxide group

INVENTOR(S):

Krishnamurthy, Sundaram; Cowan, Stanley W.

PATENT ASSIGNEE(S):

Eastman Kodak Co., USA

SOURCE:

U.S., 17 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5399467	Α	19950321	US 1993-144754	19931029
EP 653676	A1	19950517	EP 1994-203077	19941022
EP 653676	B1	19991229		
R: BE, CI	H, DE, FR	, GB, IT, LI	, NL	
JP 07181647	A2	19950721	JP 1994-264772	19941028
PRIORITY APPLN. IN	FO.:		US 1993-144754	19931029
OTHER SOURCE(S):	MA	RPAT 122:278	3041	
AB Novel photog.	Ag halid	e materials	contain dye-forming	couplers
K-NHC(O)C(R2)	(-L R)SOn	-R1 [n = 1 c]	or 2; $R2 = H$, substit	uent; R and R1
	— .			

Page 182 09530965.trn

Si(R5)2, NR5, PR5, P(O)(R5)2 and NR5SO2; (R5 = H, alkyl or aryl); and K

a coupler moiety selected from the group consisting of pyrazolone, phenol,

and naphthol]. The couplers exhibit increased coupling activity, and provide formation of dyes having improved max. magenta image dye d., contrast, and development speed.

ΙT 162849-51-6P

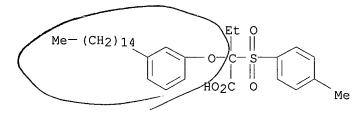
is

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (photog. couplers having ballast contg. sulfone or sulfoxide group)

RN 162849-51-6 CAPLUS

Butanoic acid, 2-[(4-methylphenyl)sulfonyl]-2-(3-pentadecylphenoxy)-CN (9CI)

(CA INDEX NAME)



ANSWER 9 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:640883 CAPLUS

DOCUMENT NUMBER: 119:240883

Metabolism of Casodex in laboratory animals TITLE:

AUTHOR(S): Boyle, G. W.; McKillop, D.; Phillips, P. J.; Harding,

J. R.; Pickford, R.; McCormick, A. D.

CORPORATE SOURCE: Saf. Med. Dep., ICI Pharm., Alderley

Park/Macclesfield/Cheshire, SK10 4TG, UK Xenobiotica (1993), 23(7), 781-98

SOURCE:

CODEN: XENOBH; ISSN: 0049-8254

DOCUMENT TYPE: Journal LANGUAGE: English

Casodex, a non-steroidal antiandrogen, was eliminated primarily in feces by rat, mouse, rabbit and dog. Rat, mouse and rabbit eliminated 20-30%

of

a single oral dose (8-25 mg/kg) in urine; only 3-4% was excreted in urine by dog (2.5 mg/kg). Oral absorption was about 80% in rat, mouse, rabbit and dog. Most of the dose was recovered in 48 h from rat, mouse and rabbit. In rat, <1% of the dose was exhaled as 14CO2 and <1% remained in the carcass after 7 days. Recovery from dog was incomplete in 4 days but consistent with the long plasma elimination half-life of 7-7.5 days. Casodex was eliminated from rat plasma with a half-life of 17-21 h. Examn. of urine indicated extensive metab. of Casodex and showed a marked species difference. In rat, mouse and dog. Casodex was cleaved at the amide to yield a carboxylic acid and an arom. amine which subsequently underwent ring hydroxylation with sulfate conjugation. In rabbit, the major urinary metabolite was Casodex glucuronide, conjugated on the tertiary hydroxyl. The major component in feces of all species was unchanged Casodex; some hydroxy-Casodex was also obsd. in rat feces. Anal. of rat and dog bile indicated that Casodex and hydroxy-Casodex were

Page 183 09530965.trn

eliminated in bile primarily as glucuronide conjugates.

151262-57-6 ΙT

RL: FORM (Formation, nonpreparative)

(formation of, as Casodex metabolite, species differences in)

RN 151262-57-6 CAPLUS

Propanoic acid, 3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) CN (CA INDEX NAME)

ANSWER 10 OF 19 CAPLUS COPYRIGHT 2002 ACS

1989:614094 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 111:214094

Chemistry of novel compounds with a multifunctional TITLE:

carbon structure. 5. Molecular design of versatile building blocks for aliphatic monofluoro molecules by

manipulation of multifunctional carbon structure

Takeuchi, Yoshio; Nagata, Kazuhiro; Koizumi, Toru AUTHOR(S): Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, CORPORATE SOURCE:

930-01, Japan

SOURCE: J. Org. Chem. (1989), 54(23), 5453-9

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal English LANGUAGE:

CASREACT 111:214094 OTHER SOURCE(S):

Three kinds of doubly functionalized monofluoromethylene fragments, PhSO2CRFNO2 (R = Me, PhCH2, CH2CO2Et, CH2CH2COMe), PhSO2CRFCO2Et (R = PhCH2, CH2CH2COMe) and O2NCRFCO2Et (I, R = PhCH2 CH2CH2CO2Et, CH2CH2COMe, CHPhCH2COMe, CH2CH2CN) potentially versatile building blocks for the

general synthesis of various aliph. monofluoro mols., were prepd. from

the

corresponding difunctional compds. by monoalkylations and selective fluorinations. The interconversion or reductive removal of each functional group followed by the introduction of the second alkyl groups

(R') at the fluorine-bearing carbon atom was examd. I proved to be

useful

and practical building blocks for conversions to the various monofluoroalkanes.

IT 122876-09-9P 122876-10-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

122876-09-9 CAPLUS RN

Benzenepropanoic acid, .alpha.-fluoro-.alpha.-(phenylsulfonyl)- (9CI) CN

(CA

INDEX NAME)

RN 122876-10-2 CAPLUS

CN Hexanoic acid, 2-fluoro-5-oxo-2-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 11 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:150945 CAPLUS

DOCUMENT NUMBER: 108:150945

TITLE: Amino acid sulfones: S-benzyl-DL-.alpha.-

methylcysteine sulfone

AUTHOR(S): Griffith, Owen W.

CORPORATE SOURCE: Med. Coll., Cornell Univ., New York, NY, 10021, USA

SOURCE: Methods Enzymol. (1987), 143(Sulfur Sulfur Amino

Acids), 274-9

CODEN: MENZAU; ISSN: 0076-6879

DOCUMENT TYPE: Journal LANGUAGE: English

AB The synthesis of S-benzyl-DL-.alpha.-methylcysteine sulfone from S-benzyl-.alpha.-methylcysteine by oxidn. is described. In addn. the reductive cleavage of the sulfone with Na/liq. NH3 to give DL-.alpha.-Me cysteinesulfonic acid is detailed. Also, a general method for the prepn. of S-benzyl derivs. of amino acids contg. thiol or disulfide groups is given.

IT 113737-61-4P, S-Benzyl-DL-.alpha.-methylcysteine sulfone

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and reductive cleavage to sulfinic acid deriv.)

RN 113737-61-4 CAPLUS

CN Alanine, 2-methyl-3-['(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER: 1987:593881 CAPLUS

DOCUMENT NUMBER: 107:193881

TITLE: Design and synthesis of phosphonate inhibitors of

glutamine synthetase

AUTHOR(S): Farrington, G. King; Kumar, Alok; Wedler, Frederick

C.

CORPORATE SOURCE: Dep. Chem., Pennsylvania State Univ., University

Park,

PA, 16802, USA

SOURCE: J. Med. Chem. (1987), 30(11), 2062-7

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:193881

AB Phosphonates, H2NCR(CO2H)CH2CH2XCH2PO3-2 (I), were designed as chem. stable analogs of the phosphorylated inhibitors, H2NCH(CO2H)CH2CH2R (R = SONHMe, SO2Me, PO3-2, etc). Phosphonates I (R = Me; X = S, SO, SO2) (II) resembled the transiently stable H2NCH(CO2H)CH2CH2SO2Me, whereas I (R =

H;

X = PO2-) (III) resembled the 2-amino-4-phosphonobutyric acid. When tested as inhibitors of glutamine synthetase (GS) from bacteria, mammals, and plants, III was proved to be the most potent, with a Ki of 7.5 .times.

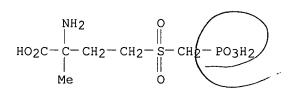
10-5 M vs. the Escherichia coli enzyme. Anal. of the inhibition data for II suggested that a replacement of the O bridging the tetrahedral S II or phosphinate III and the terminal phosphate with a hydrophobic methylene drastically reduces the enzyme's affinity for inhibitors. Enhanced affinity of GS for III may result from interaction of the neg. charge on the phosphinate with Mn2+ at the active site.

IT 110372-49-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and glutamine synthetase inhibition by)

RN 110372-49-1 CAPLUS

CN Isovaline, 4-[(phosphonomethyl)sulfonyl]- (9CI) (CA INDEX NAME)



ANSWER 13 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1985:402717 CAPLUS

DOCUMENT NUMBER: 103:2717

TITLE: The design of fluorescent probes which bind to the

active center of guanidinobenzoatase. Application to

the location of cells possessing this enzyme

AUTHOR(S): Steven, Frank S.; Griffin, Margaret M.; Al-Ahmad,

Rajaa K.

CORPORATE SOURCE: Dep. Biochem., Univ. Manchester, Manchester, UK

SOURCE: Eur. J. Biochem. (1985), 149(1), 35-40

CODEN: EJBCAI; ISSN: 0014-2956

DOCUMENT TYPE: Journal LANGUAGE: English

AB Cells possessing a known enzymic activity may be located by fluorescent probes designed to act as competitive inhibitors of this enzyme. A series

of dansyl N-substituted guanidino derivs. which bind to the active center of guanidinobenzoatase were prepd. 9-Aminoacridine also acted as a competitive inhibitor and behaved similarly to these guanidino derivs. These fluorescent probes were used to locate tumor cells possessing this enzyme in thin sections of fixed tissue by employing fluorescent microscopy.

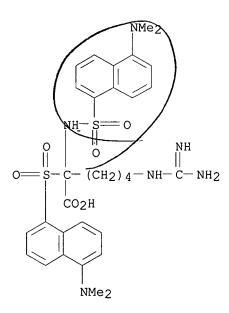
IT 96425-07-9 96425-10-4

RL: BIOL (Biological study)

(as fluorescent probe of guanidinobenzoatase active center)

RN 96425-07-9 CAPLUS

CN Lysine, N6-(aminoiminomethyl)-N2,2-bis[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]- (9CI) (CA INDEX NAME)



RN 96425-10-4 CAPLUS

CN Arginine, N2-[1-carboxy-1-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]ethyl]-2-[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]- (9CI) (CA INDEX NAME)

ANSWER 14 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1985:178450 CAPLUS

DOCUMENT NUMBER:

102:178450

TITLE:

Gas chromatographic separation of enantiomeric sulfur

compounds on Chirasil-Val

AUTHOR(S):

Bayer, Ernst; Kuesters, Ernst; Nicholson, Graeme J.;

Frank, Hartmut

CORPORATE SOURCE:

Inst. Org. Chem., Univ. Tuebingen, Tuebingen,

D-7400/1, Fed. Rep. Ger.

SOURCE:

J. Chromatogr. (1985), 320(2), 393-6 CODEN: JOCRAM; ISSN: 0021-9673

DOCUMENT TYPE:

Journal

LANGUAGE:

English

The gas chromatog. sepn. of sulfoxide antipodes, including aliph. sulfoxides, on quartz fused silica capillaries coated with the chiral silicone phase Chirasil-Val is reported. The compds. were esterified before anal. A flame ionization detector and H carrier gas were used.

IT 95833-67-3 95833-68-4

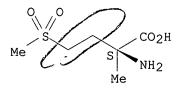
RL: ANST (Analytical study); PROC (Process)

(sepn. of, by gas chromatog. on Chirasil-Val)

RN 95833-67-3 CAPLUS

CN L-Isovaline, 4-(methylsulfonyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 95833-68-4 CAPLUS

D-Isovaline, 4-(methylsulfonyl)- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

Page 188 09530965.trn

ANSWER 15 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1981:569043 CAPLUS

DOCUMENT NUMBER:

95:169043

TITLE:

.alpha.-Amino acids as nucleophilic acyl equivalents.

V. Sterically directed Michael addition of oxazolin-5-one anions to activated double bonds;

synthesis of 1,4-dicarbonyl compounds and

.gamma.-oxonitriles

AUTHOR(S):

CORPORATE SOURCE:

Wegmann, Helmut; Steglich, Wolfgang Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300,

Fed. Rep. Ger.

SOURCE:

Chem. Ber. (1981), 114(7), 2580-94

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE:

Journal German

LANGUAGE:

GΙ

$$R^{1}$$
 O $R^{3}CH_{2}CHR^{2}$ O R^{1} N O R II

AB Reaction of oxazolinones I (R = mesityl; R1 = Me2CH, Me2CHCH2, EtMeCH) with R2CH: CHR3 [R2 = H, CN; R3 = CN, COMe, CHO, etc.; R2R3 = (CH2)3CO] in the presence of Et3N resulted in addn. exclusively at C-4 of the oxazoline

to give II, which upon hydrolysis with NaOH gave RCONHCR1(CO2H)CHR2CH2R3 (III). Oxidn. of III with Pb(OAc)4 gave R1COCHR2CH2R3.

ΙT 79137-81-8P 79137-88-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and oxidn. of, with lead tetraacetate)

RN.

79137-81-8 CAPLUS L-Leucine, 2-[2-(methylsulfonyl)ethyl]-N-(2,4,6-trimethylbenzoyl)- (9CI) CN (CA INDEX NAME)

RN 79137-88-5 CAPLUS

CN Butanoic acid, 2-(2-cyanoethyl)-4-(methylsulfonyl)-2-[(2,4,6-trimethylbenzoyl)amino]- (9CI) (CA INDEX NAME)

L5 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1972:433867 CAPLUS

DOCUMENT NUMBER:

77:33867

TITLE:

Bis-.beta.-chloroethyl sulfides. 3. Sulfones of .alpha.-chloro-.beta.-(.beta.-chloroethylthio)- and

.beta.-chloro-.alpha.-(.beta.chloroethylthio)isobutyric acid

AUTHOR(S):

Lin'kova, M. G.; Greiciute, D.; Rasteikiene, L.;

Knunyants, I. L.

CORPORATE SOURCE:

Inst. Elementoorg. Soedin., Moscow, USSR

SOURCE:

Izv. Akad. Nauk SSSR, Ser. Khim. (1972), (2), 372-6

CODEN: IASKA6

DOCUMENT TYPE:

Journal Russian

LANGUAGE:

Russian

AB C1CH2CH2CH2CMeC1CO2R [R = H (I) or Me] kept 5 days with 30% H2O2 in AcOH gave the corresponding sulfones. Similar oxidn. of a 15:85 mixt. of I and

C1CH2CH2SCMe(CH2C1)CO2H (II) gave a negligible amt. of the sulfone of II, and yielded instead C1CH2CH2SO2CH2CMeC1CO2H. This with Et3N gave CH2:CMeSO2CH2CH2Cl and eventually CH2:CMeSO2CH:CH2. Oxidn. of mixed C1CH2CH2SCH2CMeC1CO2Me and C1CH2CH2SCMe(CH2C1)CO2Me gave a mixt. contg. 75% C1CH2CMe(CO2Me)SO2CH2CH2Cl (III) and 25% C1CH2CH2SO2CH2CMeC1CO2Me. The latter and Et3N gave CH2:CHSO2CH:CMeCO2Me while the former gave CH2:CHSO2CMe(CH2C1)CO2Me. Sapon. of III with MeOH-NaOH gave CO2 and CH2:CMeSO2CH2CH2OMe. Unlike its unstable isomer, C1CH2CH2SO2CH2CMeC1CO2H

was remarkably stable and treated with SPC13 gave

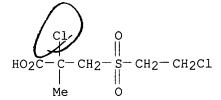
ClCH2CH2SO2CH2CMeClCOCl,

which was converted into appropriate amides with PhNH2, p-H2NC6H4CO2Me, p-H2N-C6H4CO2Et, and H2NCH(CHMe2)CO2Et0

IT 21849-24-1P

RN 21849-24-1 CAPLUS

CN Propanoic acid, 2-chloro-3-[(2-chloroethyl)sulfonyl]-2-methyl- (9CI) (CA INDEX NAME)



L5 ANSWER 17 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:488046 CAPLUS

DOCUMENT NUMBER: 75:88046

TITLE: New yperite derivatives

AUTHOR(S): Knunyants, I. L.; Kildisheva, O. V.; Lin'kova, M. G.;

Rasteikiene, L.; Greichiute, D.; Vidugiriene, V.;

Pranskiene, T.; Stumbreviciute, Z.

rialiskiene, i., Stumbevietite, z.

CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR

SOURCE: Puti Sin. Izyskaniya Protivoopukholevykh Prep.

(1970),

Volume Date 1968, No. 3, 249-56

CODEN: PSIPA4

DOCUMENT TYPE: Journal LANGUAGE: Russian

AB Yperite derivs. of the general formulas R1C(COR)ClCHMeS(CH2)2Cl (I) and R2CClHCR1(COR3)S(CH2)2Cl (II) were prepd. I were prepd. by splitting .alpha.-methyl-.alpha.-chloro-.beta.-mercaptopropionic acid .beta.-(thio lactone) with Cl followed by addn. of ethylene to give MeCl(COCl)CCH2S(CH2)2Cl. Substitution of the Cl atom in the COCl group gave I, with R1 = Cl, and R = Cl, OMe, OH, NHPh, NHCH2Ph, NHC6H4CO2Me-p, NHC6H4CO2Et-p, NHCH(CO2Et)CHMe2, and NHCH(CH2Ph)CO2Et. Also prepd. was ClCH2CH2SCH2CMe(CN)Cl. By oxidn of MeClC(CO2H)CH2S(CH2)2Cl, and carrying out similar transformations, a series of MeCCl(COR)CH2SO2(CH2)2Cl was prepd. with R = OH, Cl, OMe, NHPh, NHC6H4CO2Me-p, NHC6H4CO2-Et-p, NHCH(CH2Ph)CO2Et, and NHCH(CO2Et)CHMe2. II were obtained by addn. of .beta.-chloroethylsulfenyl chloride to acrylic, methacrylic, crotonic, cyclohexylacrylic, and cinnamic acids. II prepd. were (R1, R2, and R3 given): Me, H, Cl; Me, H, OMe; Me, H, OH; Me, H, NHPh; Me, H, NHCH2Ph;

Me,
H, NHC6H4CO2Me-p; Me, H, NHC6H4CO2Et-p; Me, H, NHCH(CO2Et)CHMe2; Me, H,
NHCH(CH2Ph)CO2Et; Me, H, NHCH(CO2H)CHMe2; Me, H, NHCH(CO2H)CH2CHMe2; Me,
H, NHCH(CH2Ph)CO2H; Me, H, NEt2; H, Me, Cl; H, Me, OH; H, Me, OEt; H, Me,
NH2; H, Me, NHPh; H, H, OEt; H, H, NHPh; and Ph, H, NH2. Also prepd. was
ClCHMeCH(CN)SCH2CH2Cl. The structures of some I and II were confirmed by
NMR spectra. On storage at room temp. most II isomerized into the
corresponding I.

IT 21849-24-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 21849-24-1 CAPLUS

CN Propanoic acid, 2-chloro-3-[(2-chloroethyl)sulfonyl]-2-methyl- (9CI) (CA INDEX NAME)

ANSWER 18 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1970:435757 CAPLUS

DOCUMENT NUMBER: 73:35757

TITLE: Amino acids containing thio ether groups and their

derivatives

INVENTOR(S): Shen, Tsung-Ying; Walford, Gordon L.; Dorn, Conrad

P.,

in

Jr.

PATENT ASSIGNEE(S): Merck and Co., Inc.

SOURCE: Brit., 20 pp.

CODEN: BRXXAA

DOCUMENT TYPE:

Patent English

LANGUAGE: Englis

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

GB 1191042 19700506

PRIORITY APPLN. INFO.: US 19670726 US 19680510

AB .beta.-Aralkylthio-substituted .alpha.-amino acids and their derivs., useful in the treatment of inflammation, are prepd. by hydrolysis of the corresponding .alpha.-amino nitriles with acids or the corresponding hydantoin compds. with alkali metal hydroxide or strong acids. Reaction of an .alpha.-substituted benzyl mercaptan with the appropriate halo-.alpha.-aminopropionic acid at elevated temp. in a polar solvent gives title compds., also prepd. by the reaction of an

.alpha.-substituted

benzyl halide with the appropriate cysteine, or by condensing an appropriate triaryl carbinol with a mercapto .alpha.-amino acid in the presence of BF3.Et20 in HOAc at elevated temp. Thus, a mixt. of 40 g 2-[tris(m-fluorophenyl)methyl-thio]butyraldehyde, 11.5 g NH4Cl, 10.4 g NaCN, 70 ml concd. aq. NH3, and 40 ml EtOH satd. with gaseous NH3 is stirred overnight at room temp. to give S-tris(m-fluorophenyl)methyl-.beta.-methyl-DL-cysteine (I). To a stirred mixt. of 6.05 g L-cysteine

150 ml refluxing liq. NH3, 15.6 g chloro(p-chlorophenyl)diphenylmethane is

added portionwise and the mixt. stirred until a clear soln. results to

give S-(p-chlorophenyldiphenylmethyl)-L-cysteine (II), m. 160-2.degree.. To a stirred mixt. of 8.4 g .beta.-bromo-.alpha.-aminopropionic acid in .apprx.150 ml refluxing liq. NH3 is added portionwise 15.5 g mercapto(p-chlorophenyl)diphenylmethane, and the mixt. stirred until a clear soln. results to give II. To a mixt. of 2.95 g p-chlorophenyldiphenylcarbinol in 10 ml HOAc and 1.5 g anhyd.

L-cysteine-HCl

at 60.degree., 1.4 ml BF3.Et20 is added. The temp. is raised to 80.degree. and the reaction allowed to continue 45 min to give II. S-Methylisothiourea sulfate (27.8 g) is added to a soln. of 26.7 g I in 100 ml 100 contg. 100 ml 100 contg. 100 ml 100 contg. 100 ml 100 ml 100 contg. 100 contg. 100 ml 100 contg. 100 con

room

temp. to give I .alpha.-guanidino-.beta.-[S-tris(m-fluorophenyl)methylthio]valeric acid. Several other examples were given. Many other compds. were cited.

IT 27446-94-2P

RN 27446-94-2 CAPLUS

CN Cystine, .beta.,.beta.'-diethyl-.alpha.,.alpha.'-bis(p-tolylsulfonyl)-, DL- (8CI) (CA INDEX NAME)

L5 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1969:77500 CAPLUS

DOCUMENT NUMBER: 70:77500

TITLE: Bis(.beta.-chloroethyl) sulfides. I. Derivatives of

.alpha.-methyl-.alpha.-chloro-.beta.-(2-

chloroethylthio)propionic and .alpha.-methyl-.alpha.-

(2-chloroethylthio) - .beta. - chloropropionic acids Greiciute, D.; Lin'kova, M. G.; Rasteikiene, L.;

Knunyants, I. L.

CORPORATE SOURCE: Inst. Elementoorg. Soedin., USSR

SOURCE: Izv. Akad. Nauk SSSR, Ser. Khim. (1968), (12),

2764-72

AUTHOR(S):

CODEN: IASKA6

DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB ClCH2CH2SCH2CMeClCOCl (I) and PhNH2 in Et2O kept 6 hrs. at -50.degree. gave the anilide, m. 35-7.degree.; benzylamine gave the N-benzylamide, m. 51-3.degree., while Et p-aminobenzoate gave 72% p-EtO2CC6H4NHCOCMe-ClCH2SCH2CH2Cl, m. 60-1.degree.; Me ester analog m. 67-8.degree.. dl-Valine Et ester in a similar reaction in the presence of Et3N in CHCl3 gave 71% EtO2CCH(CHMe2)NHCOCMeClCH2SCH2CH2Cl, m.p. unstated; dl-phenylalanine analog, an oil, was prepd. similarly. ClCH2CH2SCl and

methacrylamides in Et2O or CHCl3 gave the following ClCH2CH2SCMe (CH2Cl) COR

(R shown): NHPh, m. 35-7.degree.; NHCH2Ph, m. 54-5.degree.; NEt2, m. 65-7.degree.; p-NHC6H4CO2Me, m. 102-4.degree.; p-NHC6H4CO2Et, m. 81-3.degree.; NHCH(CH2Ph)CO2H, m. 116-18.degree.; NHCH(CHMe2)CO2H, m. 72-3.degree.; and NHCH(CH2CHMe2)CO2H, m. 94-6.degree. The yields were 51-77%. I and the theoretical amt. H2O in CHCl3 overnight gave 81% ClCH2CH2SCH2CMeClCO2H, m. 58-60.degree., also formed by addn. of ClSCH2CH2Cl to methacrylyl chloride. Oxidn. of the acid with 30% H2O2 in AcOH 10 days gave the sulfone, m. 111-13.degree., while the use of a limited amt. H2O2 overnight in the cold gave the sulfoxide, m. 98-100.degree.. The adduct of ClSCH2CH2Cl and methacrylic acid was oxidized with 30% H2O2 in AcOH to ClCH2CH2SO2CMe(CH2Cl)CO2H, m. 118-21.degree.. N.M.R. spectra of the products are shown.

IT 21849-24-1P

RN 21849-24-1 CAPLUS

CN Propanoic acid, 2-chloro-3-[(2-chloroethyl)sulfonyl]-2-methyl- (9CI) (CA INDEX NAME)

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FILE 'REGISTRY' ENTERED AT 16:59:41 ON 25 MAR 2002

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L4 97 S L1 FUL

FILE 'CAPLUS' ENTERED AT 17:00:39 ON 25 MAR 2002

L5 19 S L4

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LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 88.43 229.12 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL SESSION ENTRY CA SUBSCRIBER PRICE -11.77 -11.77

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Connection closed by remote host

DOCUMENT NUMBER: 129:244921

TITLE: Preparation of aromatic sulfonyl alpha-hydroxy

hydroxamic acid compounds as matrix metalloprotease

inhibitors

INVENTOR(S): Freskos, John N.; Boehm, Terri L.; Mischke, Brent V.;

Heintz, Robert M.; Mcdonald, Joseph J.; Decrescenzo,

Gary A.; Howard, Susan C.

PATENT ASSIGNEE(S):

SOURCE:

Monsanto Company, USA PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.			KIND DATE					APPLICATION NO.					DATE				
	WO	9839326			A1 19980911				WO 1998-US4277				19980304					
		W:	AL,	AU,	BA,	BB,	BG,	BR,	CA,	CN	CU,	CZ,	EE,	GE,	GH,	GW,	HU,	ID,
			IL,	IS,	JP,	KP,	KR,	LC,	LK,	LR	LT,	LV,	MG,	MK,	MN,	MX,	NO,	ΝZ,
			PL,	RO,	SG,	SI,	SK,	SL,	TR,	TT.	, UA,	US,	UZ,	VN,	YU,	AM,	ΑZ,	BY,
			KG,	ΚZ,	MD,	RU,	ТJ,	TM										•
		RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	DE,	DK,	ES,	FI,
			FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,
			GΑ,	GN,	ML,	MR,	ΝE,	SN,	TD,	ΤG								
	ΑU	9864	478		A.	1 :	1998	0922		Ž	AU 19	98-6	4478		19980	304		
	ŪΑ	7373	29		B:	2 :	2001	0816										
	EΡ	9849	59		A.	1 :	2000	0315		I	EP 19	98-9	1017	7	19980	0304		
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	PT,	ΙE,
FI																		
	BR	98083	150		Α		2000	0328		I	3R 19	98-8	150		19980	0304		
PRIO	RITY	APP	LN.	INFO	. :				1	US :	1997-	3518	2 P	P	19970	0304		
									1	WO :	1998-	US42	77	W	19980	0304		

OTHER SOURCE(S): MARPAT 129:244921

AB The title compds. HONHC(O)C(OH)(R2)CH2SO2R1 [I; R2 = H, C1-4 alkyl, C1-4 haloalkyl, etc.; R1 = 5-6 membered cycloalkyl, heterocyclyl, aryl, etc.] which inter alia inhibit matrix metalloprotease activity, were prepd. Thus, multi-step synthesis of I [R1 = 4-PhOC6H4; R2 = Me] which showed 51.9% inhibition of angiogenesis in the cornea of a mouse, was described.

IT 213184-20-4P 213184-29-3P 213184-51-1P 213184-61-3P 213184-63-5P 213184-65-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of arom. sulfonyl alpha-hydroxy hydroxamic acid compds. as matrix metalloprotease inhibitors)

RN 213184-20-4 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[(4-phenoxyphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Page 180

09530965.trn

RN 213184-29-3 CAPLUS

CN Propanoic acid, 3-[[4-(3,4-dimethylphenoxy)phenyl]sulfonyl]-2-hydroxy-2-methyl- (9CI) (CA INDEX NAME)

RN 213184-51-1 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[(4-nitrophenyl)sulfonyl]- (9CI)

(CA

INDEX NAME)

RN 213184-61-3 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX

NAME)

RN 213184-63-5 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[[4-[[[(3-

 $\label{lem:methylphenyl} $$ methylphenyl] amino] phenyl] sulfonyl] - (9CI) (CA INDEX NAME)$

RN 213184-65-7 CAPLUS

CN Propanoic acid, 2-hydroxy-2-methyl-3-[[4-[[(4-

methylphenyl)amino]carbonyl]amino]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

ANSWER 8 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER:

1995:532307 CAPLUS

DOCUMENT NUMBER:

122:278041

TITLE:

Photographic couplers having a ballast containing a

sulfone or sulfoxide group

INVENTOR(S):

Krishnamurthy, Sundaram; Cowan, Stanley W.

PATENT ASSIGNEE(S):

SOURCE:

Eastman Kodak Co., USA U.S., 17 pp.

CODEN: USXXAM

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5399467	A	19950321	US 1993-144754	19931029
EP 653676	A1	19950517	EP 1994-203077	19941022
EP 653676	B1	19991229		
R: BE, CH,	DE, FR	, GB, IT, LI,	NL	
JP 07181647	A2	19950721	JP 1994-264772	19941028
PRIORITY APPLN. INFO	. :		US 1993-144754	19931029
OTHER SOURCE(S):	MA	RPAT 122:2780	041	
AB Novel photog. Ac	g halid	e materials o	contain dye-forming	couplers
K-NHC(O)C(R2)(-1	L R)SOn	-R1 [n = 1 or	2; $R2 = H$, substit	uent; R and R1 =
substituent; L	is sele	cted from the	e group consisting o	of O, S, Se, Te,

09530965.trn

Page 182

Si(R5)2, NR5, PR5, P(0)(R5)2 and NR5SO2; (R5 = H, alkyl or aryl); and Kis

a coupler moiety selected from the group consisting of pyrazolone, phenol,

and naphthol]. The couplers exhibit increased coupling activity, and provide formation of dyes having improved max. magenta image dye d., contrast, and development speed.

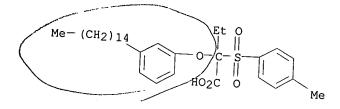
IT 162849-51-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (photog. couplers having ballast contg. sulfone or sulfoxide group) 162849-51-6 CAPLUS

RN CN

Butanoic acid, 2-[(4-methylphenyl)sulfonyl]-2-(3-pentadecylphenoxy)-(9CI)

(CA INDEX NAME)



ANSWER 9 OF 19 CAPLUS COPYRIGHT 2002 ACS ACCESSION NUMBER:

1993:640883 CAPLUS DOCUMENT NUMBER:

119:240883 TITLE:

Metabolism of Casodex in laboratory animals AUTHOR(S):

Boyle, G. W.; McKillop, D.; Phillips, P. J.; Harding,

J. R.; Pickford, R.; McCormick, A. D. CORPORATE SOURCE:

Saf. Med. Dep., ICI Pharm., Alderley

Park/Macclesfield/Cheshire, SK10 4TG, UK Xenobiotica (1993), 23(7), 781-98 SOURCE:

CODEN: XENOBH; ISSN: 0049-8254

DOCUMENT TYPE: Journal LANGUAGE: English

Casodex, a non-steroidal antiandrogen, was eliminated primarily in feces by rat, mouse, rabbit and dog. Rat, mouse and rabbit eliminated 20-30% of

a single oral dose (8-25 mg/kg) in urine; only 3-4% was excreted in urine by dog (2.5 mg/kg). Oral absorption was about 80% in rat, mouse, rabbit and dog. Most of the dose was recovered in 48 h from rat, mouse and rabbit. In rat, <1% of the dose was exhaled as 14CO2 and <1% remained in the carcass after 7 days. Recovery from dog was incomplete in 4 days but consistent with the long plasma elimination half-life of 7-7.5 days. Casodex was eliminated from rat plasma with a half-life of 17-21 h. Examn. of urine indicated extensive metab. of Casodex and showed a marked species difference. In rat, mouse and dog. Casodex was cleaved at the amide to yield a carboxylic acid and an arom. amine which subsequently underwent ring hydroxylation with sulfate conjugation. In rabbit, the major urinary metabolite was Casodex glucuronide, conjugated on the tertiary hydroxyl. The major component in feces of all species was unchanged Casodex; some hydroxy-Casodex was also obsd. in rat feces. Anal. of rat and dog bile indicated that Casodex and hydroxy-Casodex were

09530965.trn

Page 183

eliminated in bile primarily as glucuronide conjugates. ΙT 151262-57-6

RL: FORM (Formation, nonpreparative)

(formation of, as Casodex metabolite, species differences in)

RN 151262-57-6 CAPLUS

Propanoic acid, 3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methyl- (9CI) CN

ANSWER 10 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: DOCUMENT NUMBER:

1989:614094 CAPLUS

111:214094

TITLE:

Chemistry of novel compounds with a multifunctional carbon structure. 5. Molecular design of versatile building blocks for aliphatic monofluoro molecules by manipulation of multifunctional carbon structure

AUTHOR(S):

Takeuchi, Yoshio; Nagata, Kazuhiro; Koizumi, Toru CORPORATE SOURCE: Fac. Pharm. Sci., Toyama Med. Pharm. Univ., Toyama, 930-01, Japan

SOURCE:

J. Org. Chem. (1989), 54(23), 5453-9

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S):

CASREACT 111:214094 Three kinds of doubly functionalized monofluoromethylene fragments, PhSO2CRFNO2 (R = Me, PhCH2, CH2CO2Et, CH2CH2COMe), PhSO2CRFCO2Et (R = PhCH2, CH2CH2COMe) and O2NCRFCO2Et (I, R = PhCH2 CH2CH2CO2Et, CH2CH2COMe,

CHPhCH2COMe, CH2CH2CN) potentially versatile building blocks for the general synthesis of various aliph. monofluoro mols., were prepd. from

the

corresponding difunctional compds. by monoalkylations and selective fluorinations. The interconversion or reductive removal of each functional group followed by the introduction of the second alkyl groups (R') at the fluorine-bearing carbon atom was examd. I proved to be useful

and practical building blocks for conversions to the various

122876-09-9P 122876-10-2P IT

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 122876-09-9 CAPLUS

Benzenepropanoic acid, .alpha.-fluoro-.alpha.-(phenylsulfonyl)- (9CI) CN (CA

INDEX NAME)

RN 122876-10-2 CAPLUS

Hexanoic acid, 2-fluoro-5-oxo-2-(phenylsulfonyl)- (9CI) (CA INDEX NAME) CN

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:150945 CAPLUS

DOCUMENT NUMBER: 108:150945

TITLE: Amino acid sulfones: S-benzyl-DL-.alpha.-

methylcysteine sulfone

AUTHOR(S): Griffith, Owen W.

CORPORATE SOURCE: Med. Coll., Cornell Univ., New York, NY, 10021, USA SOURCE:

Methods Enzymol. (1987), 143(Sulfur Sulfur Amino

Acids), 274-9

CODEN: MENZAU; ISSN: 0076-6879

DOCUMENT TYPE: Journal

LANGUAGE: English

The synthesis of S-benzyl-DL-.alpha.-methylcysteine sulfone from S-benzyl-.alpha.-methylcysteine by oxidn. is described. In addn. the reductive cleavage of the sulfone with Na/liq. NH3 to give DL-.alpha.-Me cysteinesulfonic acid is detailed. Also, a general method for the prepn. of S-benzyl derivs. of amino acids contg. thiol or disulfide groups is

113737-61-4P, S-Benzyl-DL-.alpha.-methylcysteine sulfone IT RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and reductive cleavage to sulfinic acid deriv.)

RN 113737-61-4 CAPLUS

Alanine, 2-methyl-3-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME) CN